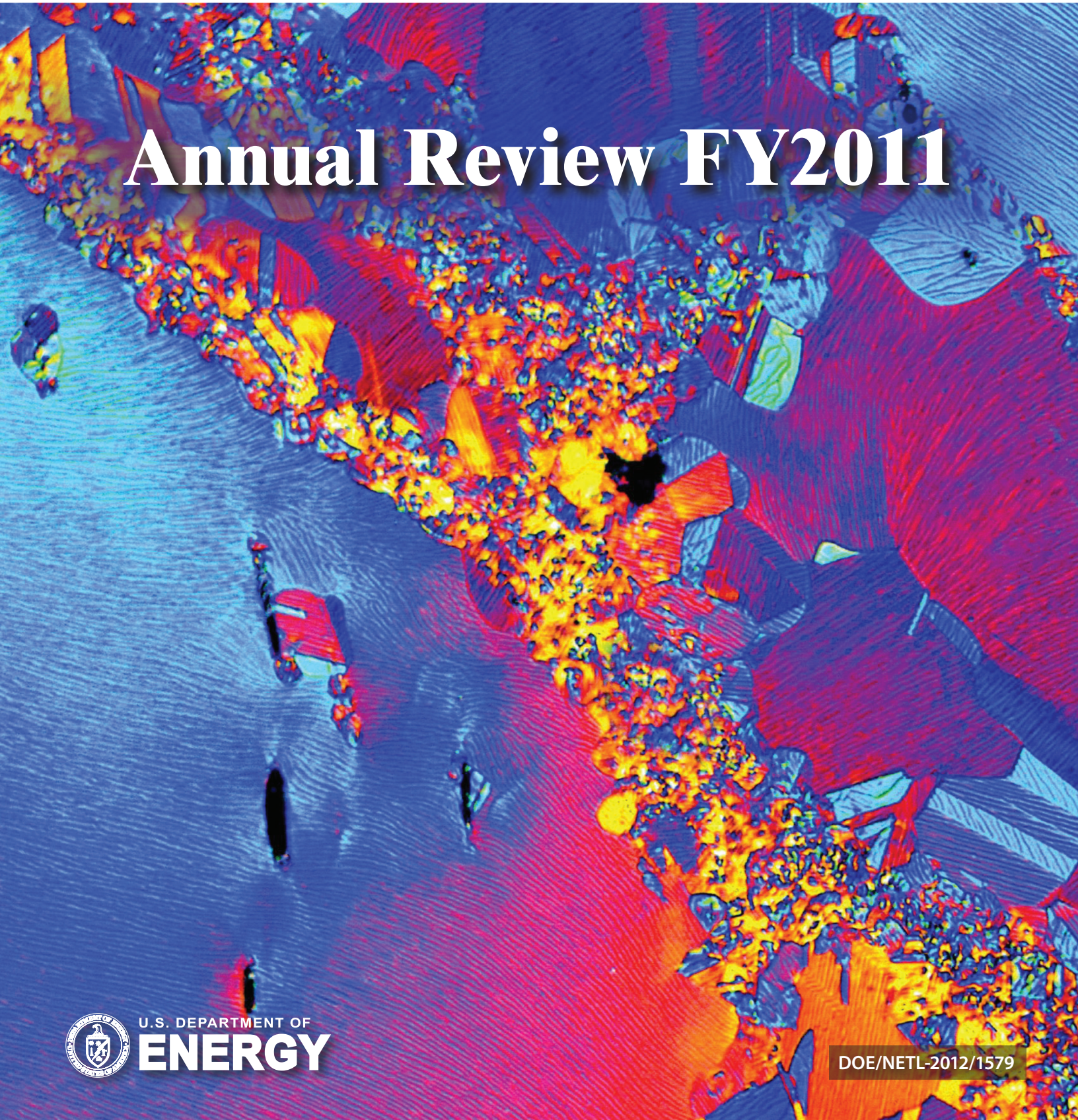
NETL-RUA

Regional University Alliance

Annual Review FY2011



U.S. DEPARTMENT OF ENERGY

DOE/NETL-2012/1579

Disclaimer

Front Cover:

Photo micrographic image of a platinum chromium (PtCr) alloy developed at NETL. This new alloy won an R&D100 award and a Federal Laboratory Consortium (FLC) Far West Region award in 2011 and a FLC national award in 2012. A new coronary stent, which incorporates this innovative metal alloy, is more flexible and comfortable than traditional stainless steel stents and is more visible on the X-rays of a patient. The stent, designed and marketed by Boston Scientific has achieved more than $4 billion in sales and captured a 45 percent share of domestic and about 30% of world coronary stent markets.

NETL-REGIONAL UNIVERSITY ALLIANCE
Annual Review FY2011

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FINAL REPORT

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National Energy Technology Laboratory

www.netl.doe.gov

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Acknowledgments

The efforts described in this report were made possible through the funding and guidance provided by the NETL Strategic Center for Coal and Strategic Center for Natural Gas and Oil. The guidance and support of NETL Office of Research and Development senior management and the NETL-RUA Executive Committee were crucial to the success of these research efforts.

The contents of this report reflect the hard work and dedication of a multitude of researchers from NETL and its five university alliance, which was made possible through DOE NETL contract No. DE-FE0004000.

Support provided under DOE Contract No. DE-FE0004003 for the preparation of this report is gratefully acknowledged.

Table of Contents

Abbreviations

ANSYS-FLUENT	a multiphase CFD solver
APECS	Advanced Process Engineering Co-simulator
AVESTAR™	Advanced Virtual Energy Simulation Training and Research
C2U	Carbon Capture Unit
C3M™	Carbonaceous Chemistry for Computational Modeling
CAL	Consortium Area Lead (university)
Carnegie Mellon	Carnegie Mellon University
CCS	carbon capture and storage
CCSI	Carbon Capture Simulation Initiative
CCU (or C_2U)	Carbon Capture Unit
CFD	computational fluid dynamics
CLR	chemical looping reactor
CMRA	Critical Materials Research Alliance
CMU	Carnegie Mellon University
CNT	carbon nanotube
CPD	devolatilization software
CRADAs	cooperative research and development agreements
DEM	discrete element method
DEXA	dual-energy x-ray absorptionmetry
DOE	United States Department of Energy
FAL	Focus Area Lead (federal)
FAM	Focus Area Manager (contractor)
FG-FVC	a coal kinetic database
FLC	Federal Laboratory Consortium
FRTG	(National Incident Command) Flow Rate Technical Group
FPU	Fuel Processing Unit
FY	fiscal year
GTC	Grid Technologies Collaborative
ICMI	Industrial Carbon Management Initiative
ICP-OES	inductively coupled plasma optical emission spectroscopy
IGCC	integrated gasification combined cycle
IIA	inter-institutional agreements
ILs	ionic liquids
ITS	immersive training system
LIBS	laser induced breakdown spectroscopy
MC-ICP-MS	multi-collector – inductively coupled plasma - mass spectrometer
MFIX	a multiphase CFD solver
MOF	metal organic framework

MOSS	members only sharepoint site
MOU	memorandum of understanding
NDA	non-disclosure agreement
NETL	National Energy Technology Laboratory
NETL-RUA	National Energy Technology Laboratory-Regional University Alliance
NIST	National Institute for Standards and Testing
NRAP	National Risk Assessment Partnership (NRAP)
NRCCE	National Research Center for Coal and Energy
ORD	Office of Research and Development
ORISE	Oak Ridge Institute for Science and Education
OSU	Oregon State University
OTS	operator training system
PACS	Professional Analytical and Consulting Services, Inc.
Penn State	Pennsylvania State University
PC	pulverized coal
PI	principal investigator
Pitt	University of Pittsburgh
QMVA	quantitative monitoring, verification and accounting
R&D	research and development
RES	Research and Engineering Services
ROM	reduced order model
SATC	Associacao Beneficente da Industria Carbonifera de Santa Catarina/Coal Mining Industry Beneficent Association from Santa Catarina
SBEUC	Simulation Based Engineering User Center
SCC	Strategic Center for Coal
SCNGO	Strategic Center for Natural Gas and Oil
SGA	strategic growth area
SOFC	solid oxide fuel cell
SPE	Society of Petroleum Engineers
TGA	thermogravimetric analysis
UEP	University Energy Partnership
URS	URS Corporation
USBM	United States Bureau of Mines
USGS	United States Geological Survey
UTC	United Technologies Corporation
VCU	Virginia Commonwealth University
Virginia Tech	Virginia Polytechnic Institute and State University
WVU	West Virginia University

“Coming together is a beginning.
Keeping together is progress.
Working together is success.”

—Henry Ford

A Word from NETL'S Director of Office of Research and Development

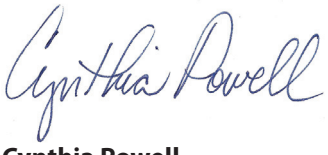
Cynthia Powell, Director, NETL Office of Research and Development

On October 13, 2010, the National Energy Technology Laboratory celebrated a hundred years of fossil energy research in support of the nation's domestic energy security, and stepped into a new era of research collaboration and innovation with the official launch of the NETL-Regional University Alliance for Energy Innovation. The NETL-RUA is an alliance comprising NETL's Office of Research & Development, URS Corporation, and five regional universities—Carnegie Mellon University, Penn State, the University of Pittsburgh, Virginia Tech, and West Virginia University—dedicated to discovering, developing, and deploying advanced energy technologies that enable sustainable utilization of the nation's domestic energy resources.

In the following pages you will find a summary of the work that we did together in fiscal year 2011, the first full year of our partnership. The NETL-RUA 2011 research portfolio spanned the fossil energy gamut from advanced energy systems, to carbon capture, to carbon utilization and storage, to unconventional resources like ultra-deep oil and methane hydrates. For every research project, we pulled together a multi-organizational team that leveraged the best that each organization has to offer, to overcome the barriers that limit sustainable, affordable utilization of our nation's energy resources. Federal and URS scientists and engineers worked side-by-side with university faculty, students and post-docs to discover and test new materials concepts; develop and verify higher performance energy systems; create new algorithms and models that will speed technology development and enhance scientific understanding; and deploy new technologies in the field. In the process, we managed to win several prestigious awards, add a number of articles to the scientific literature, and mentor 131 young people who will be among our energy leaders of tomorrow.

Our research partnership is still evolving, but I think that you will agree that 2011 was a very successful first year for the NETL-RUA. I am very pleased and proud to be part of this endeavor, and I look forward to a time in the not-too-distant future when the NETL-RUA is recognized regionally, nationally, and globally as a respected energy research partnership.

Respectfully,



Cynthia Powell
Director
Office of Research and Development
National Energy Technology Laboratory

Letter from NETL-RUA Manager

Julianne Klara,
NETL-RUA Manager

Tackling carbon management and securing sources of sustainable energy are enduring priorities of the National Energy Technology Laboratory Regional University Alliance (NETL-RUA) and are arguably the most pressing issues facing us today. The NETL-RUA has worked over this past year to establish new and more effective strategies to collaborate on research, development, and demonstration programs to tackle these challenges. The integration of regional capabilities and the extraordinary energy expertise offered by the alliance uniquely positions NETL-RUA to develop transformative science and technology solutions to transition to a low-carbon energy future.

F2011 marked a significant milestone in the maturation of the NETL-RUA. Under the direction of its Executive Committee, the NETL-RUA agreed to jointly fund several key initiatives in areas that represent significant opportunities for growth. Though some of these areas represent markets "adjacent" to the core fossil energy research portfolio, these areas are relevant for a coherent transition from a fossil-based economy to a sustainable energy future. For these growth initiatives, the traditional NETL-RUA research model, which relies solely on NETL sponsorship with funding nearly exclusively from DOE's Office of Fossil Energy, shifted to a new model that draws on guidance and funding collectively provided by all NETL-RUA member organizations.

The NETL-RUA has also implemented initiatives to forge stronger relationships with the commercial sector and develop joint projects with sister DOE laboratories. Advancing these partnerships will position NETL-RUA to better serve as a source of regional economic development and nationwide job creation.

Further, our continued engagement of students at both the undergraduate and graduate level in cutting-edge energy research provides hands-on experience in multi-disciplinary areas of science, technology and entrepreneurship. Development of these energy leaders is providing the expertise and experience that industry can and will rely on for the future.

Significant progress has also been achieved this year to increase the visibility and impact of NETL-RUA with the establishment of the NETL-RUA website, through various media outreach campaigns and events, and the issuance of a monthly NETL-RUA eNews newsletter. We have identified improvements to the efficiency and effectiveness of our operations and continue to evaluate, assess and improve our ways of working and, most importantly, remain open to new ideas to take the NETL-RUA into the future.

Henry Ford said, "Coming together is a beginning. Keeping together is progress. Working together is success." As the highlights listed in this report illustrate, the NETL-RUA is beginning to reap the rewards of its members successfully working together. The achievements listed in this review would not have been possible without the commitment of our federal, university and industry partner researchers.

Having adapted to the challenges presented in fiscal year 2011, we are fully prepared to continue the strive toward achievement of our vision in the year to come. We look forward to an even more successful year for 2012!

Respectfully,

Julianne M. Klara
NETL-RUA Manager
Office of Research and Development
National Energy Technology Laboratory

FY2011
NETL-RUA Executive Committee

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Vice President for Research
Pennsylvania State University

Pradeep Khosla
Dean of Engineering
Carnegie Mellon University

Julianne Klara
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Cynthia Powell (Committee Chair)
Director, Office of Research and Development
National Energy Technology Laboratory

Robert Walters
Vice President for Research
Virginia Polytechnic Institute and State University

Christina Gabriel (ex officio)
President
University Energy Partnership

The Year in Review

The NETL-RUA

FY2011 marks the first full year of operation of the NETL-RUA. The NETL-RUA combines the facilities, expertise, and resources of the National Energy Technology Laboratory (NETL) with those of Carnegie Mellon University (CMU), Pennsylvania State University (Penn State), the University of Pittsburgh (Pitt), Virginia Polytechnic Institute and State University (Virginia Tech), and West Virginia University (WVU), as well as industry partner URS Corporation, one of the nation's largest and most comprehensive engineering services firms.

The NETL-RUA was formed to leverage the talent and resources of these regional universities, strengthen NETL research efforts for energy and energy-related environmental systems development, provide greater regional and national impact through job creation, and facilitate training for the next generation of scientists and engineers.

These efforts will in turn bolster the U.S. scientific community's ability to address future challenges associated with energy supply, reliability, sustainability, and environmental impact that will affect the nation and world.

Whereas much of FY2010 was spent inventorying the collective capabilities of the member organizations and structuring research teams with the right expertise to address the Fossil Energy mission, FY2011 focused on improving the collaborative dynamics of the seven member partnership, identifying and investigating new opportunities to grow the research portfolio, and increasing the NETL-RUA's economic and technological impact.

Key Research Accomplishments

This report describes the accomplishments achieved through this collaborative research effort and the significant progress that has been made.

NETL-RUA researchers are daily making discoveries and developing technology to keep energy and power production secure and affordable while reducing air emissions, water pollution, and land use.

The NETL-RUA "promises advanced energy technologies and growth in our regional and national economies. It promises high-tech jobs for our nation's engineers and scientists. And it promises the education of a new generation of researchers and entrepreneurs who are passionate about pursuing sustainable energy sources for our children and our children's children."

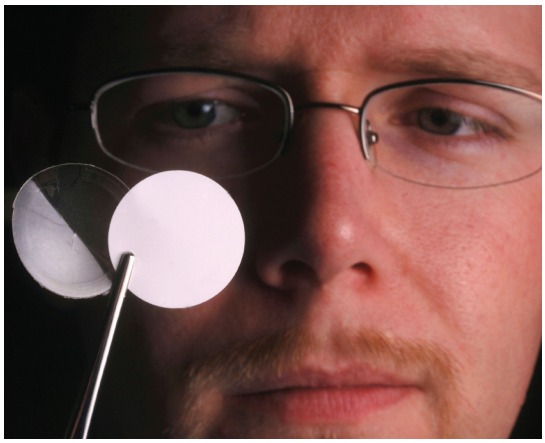
—Anthony Cugini, October 2010.

Reducing the CO_2 Footprint

Reducing carbon emissions from fossil-fueled power plants can be accomplished through various options including optimized designs to improve process efficiency, CO_2 separation and capture, and CO_2 utilization. To accomplish this, NETL-RUA researchers are developing high performance materials for system components; highly selective, lower-cost sorbents, solvents and membranes; and novel CO_2 conversion processes.

Further, continued use of fossil fuels is dependent on the ability to safely and permanently store CO_2 over long periods of time. NETL-RUA research efforts are increasing our understanding of CO_2 storage technology including CO_2 migration, revealing potential issues, and providing remedies for leakage and more accurate estimates for long-term storage potential.

- Discovered a composite ionic liquid and carbon nanotube material with improved CO_2 capture solvent properties.
- Validated a computational approach to accurately characterize the interaction of CO_2 with photo-catalytic materials that can be exploited to improve performance in larger scale systems.
- Developed and demonstrated novel structurally dynamic metal organic frameworks (MOFs) that selectively absorb CO_2 from mixed gas streams containing N_2 and CH_4.
- Successfully cast a superalloy for use in the high-temperature and high-pressure environment of ultra-supercritical steam boilers and turbines.
- Verified and studied the evolution of corrosion products of hydrogen separation materials to design new and better separation materials for harsh "real" syngas environments.
- Identified and tested novel cathode architectures that exhibited significantly improved capacity for energy storage applications.
- Tested and characterized dry CO_2 sorbents that can avoid the significant energy penalty associated with solvent-water vaporization in conventional flue gas scrubbing systems.
- Experimentally measured oxygen carrier performance as a function of operating conditions, composition, and morphology to determine the potential of chemical looping as a new CO_2 capture approach.

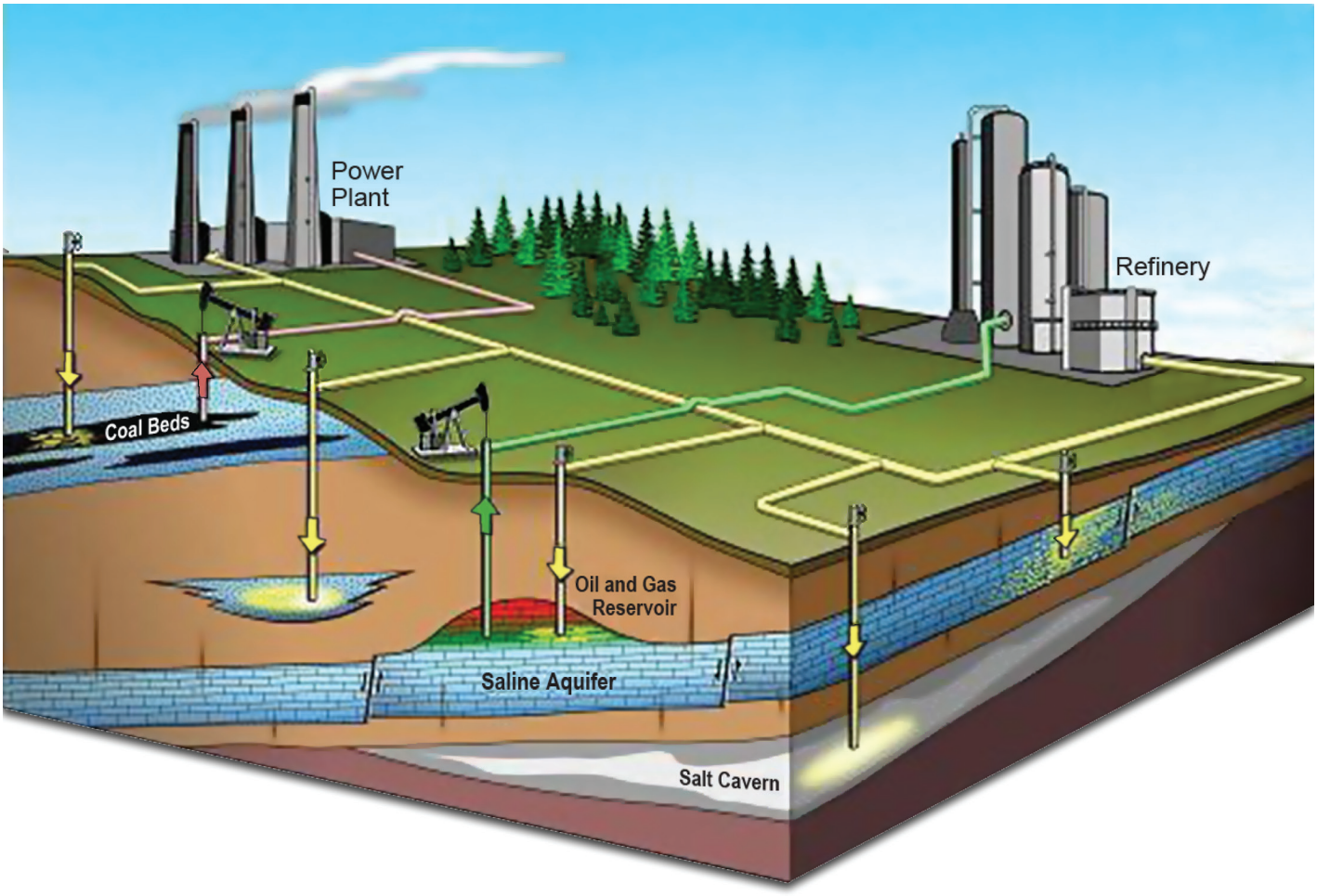


Gas Separation Membranes—Membranes have potential to purify CO_2 without process changes or energy input.

- Provided experimental evidence of chemical self-sealing behavior in damaged wellbore cement under a range of simulated deep CO_2 storage conditions.

- Developed an improved methodology for estimating CO_2 storage potential.

- Demonstrated that natural isotopic tracers can be used to differentiate sources of potential groundwater impacts.



Captured CO_2 from utilities and industrial operations can be stored in underground formations.

Accelerating Development and Deployment of Energy Technology

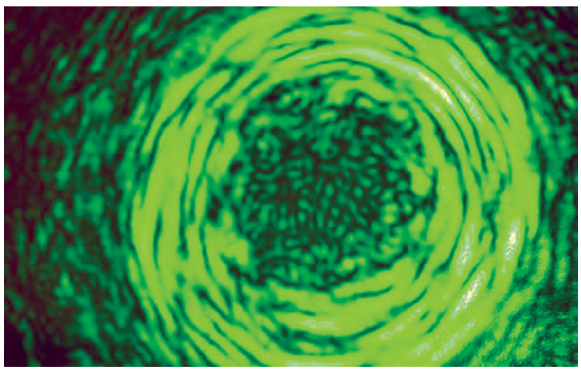
By combining experimentation and computational modeling, it is possible to accelerate development and deployment of technology by more rapidly screening potential concepts, optimizing system performance, eliminating some scale-up design and testing, and ultimately reducing the risk of commercial deployment. Computer simulations and models can also be used as training tools in the operation and maintenance of advanced energy plants.

- Established the Advanced Virtual Energy Simulation Training and Research (AVESTAR™) Center with the deployment of a first-of-a-kind integrated gasification combined cycle (IGCC) dynamic simulator.
- Advanced capabilities permitted, for the first time, the simulation of multiphase flow behavior of gas-solid flows.
- Launched the CCSI to develop a simulation toolset that enables the rapid development and deployment of new carbon capture technologies.
- Licensed the Carbonaceous Chemistry for Computational Modeling (C3M™) software.

Protecting Human Health and the Environment

NETL has been instrumental in developing technologies that reduce emissions of sulfur, NO_X, and particulate matter. Increasingly stringent emission regulations for fossil-based electric generation and improved process control require the ability to quickly and cost-effectively measure gas composition and trace contaminants.

- Developed and demonstrated a new gas analyzer package that uses fiber optics and Raman light-scattering to analyze the composition of gas streams in less than one second, with accuracy comparable to or better than existing approaches.



NETL scientists are constructing extremely fast and accurate Raman gas sensors for measuring hydrocarbon gases and other mixtures of scientific interest.

Ensuring Energy Security

The safe and clean production of affordable, domestic unconventional fossil energy resources can reduce our dependence on foreign sources of fuel. NETL-RUA research efforts have improved our ability to understand the behavior of these systems and the impacts and issues associated with production of the resource.

- Developed improved equations of state that more accurately model hydrocarbon fluids under the extreme conditions within the reservoir.
- Spearheaded a public-private collaboration to document environmental baselines and changes resulting from shale-gas development.
- Confirmed experimentally that methane hydrate reformation during gas production is a potential impediment to continuous gas production from a reservoir.

Addressing issues related to accurate methane measurements during upstream gas development.

Research Recognition

FY2011 proved to be an award-winning year for NETL-RUA researchers and the exceptional work they do. A good measure of the impact of NETL-RUA research efforts is the number and breadth of awards garnered from outside organizations that objectively compare NETL-RUA research against that of peer organizations and researchers. By that measure, NETL-RUA can be proud of its recognition as a research and technology innovator where "energy challenges converge and energy solutions emerge."

R&D 100 Awards

R&D 100 awards recognize the 100 most technologically significant products to enter the market place in a given year. In FY2011, NETL-RUA researchers were awarded three of these prestigious awards for the following:

- Manganese-Cobalt SOFC Interconnect Coating
- Advanced Process Engineering Co-simulator (APECS)v2.0 with ANSYS DesignExplorer and Rom Builder
- Novel Platinum/chromium Alloy for Improved Coronary Stent

2011 Activated Carbon Hall of Fame Award

This award, sponsored by Professional Analytical and Consulting Services, Inc. (PAC), is bestowed upon an individual for performing outstanding work that benefits the activated carbon industry. Evan Granite (NETL) was the 2011 recipient for his work on recovery of mercury from water and air.

Gustav Elrich Award

The Gustav Elrich Award was established to recognize outstanding young researchers in the field of refractory materials development. The 2011 award recipient was Jinichiro Nakano (URS) for his NETL-RUA research on thermodynamic modeling of coal-petcoke slag composition and its impact on gasifier refractories.

SPE International Best Paper Award

Dustin McIntyre (DOE), Jinesh Jain (URS), Shameem Siddiqui (Texas Tech), Krishna Ayyalasomayajula (ORISE), and J.P. Singh and Fan Yu-Yueh (Mississippi State) were awarded best paper for "Analysis of Calibration Materials to Improve Dual-Energy CT Scanning for Petrophysical Applications".

U.S. Secretary of Energy Achievement Awards and USGS Director's Award for Exemplary Achievement

NETL-RUA teams of experts were called upon to answer important questions, under difficult time constraints and during a period of intense public scrutiny, about the amount of oil leaking from the Macondo Well. In recognition for their exemplary service to the nation, the Flow Rate Technical Group (FRTG) and other NETL and partner agency teams were honored with awards from both the United States Geological Survey (USGS) and the Department of Energy (DOE).

The National Energy Technology Laboratory received a second Department of Energy Secretary Achievement Award for its role in DOE's remediation activities at the Hanford nuclear materials production site in Washington State. An NETL-RUA team of computational fluid dynamics scientists evaluated design specifications for a pulse-jet mixing vessel under development at the site. The mixer must safely process 53 million gallons of liquid nuclear waste as it changes into a stable glass form for permanent storage. The team received the award from Energy Secretary Stephen Chu. It is the highest nonmonetary award that a DOE team can receive from the Department.

NETL-RUA Strategic Priorities

Strategic Priorities

Our nation's energy security is dependent on next-generation energy technologies that combine affordability and reliability with long-term environmental stewardship and sustainability.

By most accounts, fossil fuels are projected to remain a cornerstone of our energy production and economy for the near future. Continued use of these fuels will require innovative technology to reduce emissions of greenhouse gases, air pollutants, and waste streams, and also minimize water and land use and protect our natural resources.

The NETL-RUA is poised to address fossil fuel-related issues while also developing the technologies that will allow a smooth transition to next-generation energy systems. To accomplish this, the NETL-RUA will draw on the multifaceted, collaborative research efforts of experts from the National Energy Technology Laboratory; five nationally and internationally renowned universities; and URS, one of the nation's largest engineering and site-support contractors.

NETL, its academic colleagues, and industry have a nearly 100-year history of partnering to solve the nation's energy issues by developing and commercializing new technologies.

The NETL-RUA is capitalizing on these historical relationships and the energy innovators that make up this Alliance to establish a mission focused on ensuring a robust energy future and grounded in a set of aggressive strategic goals.

Computational screening to more quickly identify promising concepts is at the heart of the NETL-RUA's research model.

NETL-RUA Strategic Priorities:

1. Perform innovative, collaborative research to meet U.S. demand for energy, power, fuels, and chemicals from fossil fuels and allow for a smooth transition to a sustainable energy future
2. Increase the economic impact of the R&D portfolio through new opportunities and markets
3. Accelerate commercialization of advanced technologies through cooperative programs
4. Prepare tomorrow's energy leaders

Mission

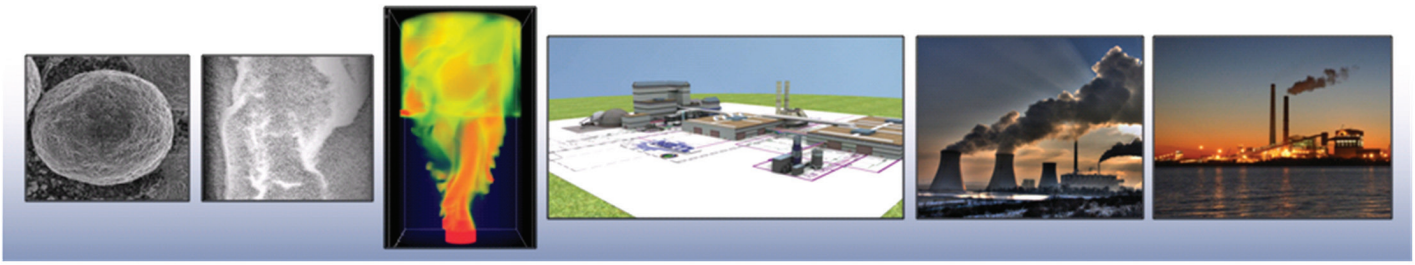
The mission of the NETL-RUA is to develop deployable energy and environmental technologies for fossil energy and to ensure a robust energy future through:

- Developing the basic science and advanced technologies to meet U.S. demand for energy, power, fuels, and chemicals
- Accelerating the validation of new concepts by providing researchers with access to signature research facilities for a range of energy applications
- Driving the commercialization viability of technologies developed through cooperative programs
- Promoting economic development by using advanced technologies as the impetus for spin-off industries
- Educating and preparing the nation's future energy leaders

Validating computational models through bench-scale experimentation can reduce design-time, enhance troubleshooting, and result in optimal science-based system designs.

Quantifying and reducing the technical risk of expanding from laboratory to commercial-scale and replacing some physical operational tests with virtual plant simulations helps to stabilize deployment costs and accelerate commercial deployment of innovative technologies.

This approach relies on academia, NETL, and industry partnering to take a concept from basic principles through proof-of-concept and component testing in lab and real-world environments to, ultimately, pilot testing, demonstration, and commercial operation.



Science-Based Prediction to Accelerate Commercialization.

Strategic Priority #1:

Perform Innovative Research

Develop advanced energy systems based on sound science and consistent with the sustainable use of energy and environmental resources to meet present and future challenges in the production of energy, power, fuels, and chemicals.

Core Fossil Energy Research

Plentiful energy supplies underpin an increased standard of living, promote energy security, and improve global collaboration.

Energy infrastructures are highly complex, interconnected, and continually evolving in response to changes in environmental constraints, economic pressures, and energy demand.

Advanced energy systems based on sound science and consistent with the sustainable use of energy and environmental resources are key to meeting the present and future needs of our global society for power, chemicals, and food.

The focus of NETL-RUA research and development is to discover and develop technologies to transform fossil energy into a clean, sustainable domestic resource.

Top researchers from all of the member organizations are collaborating to assess the current state of the science, identify grand challenges, and support efforts to match technology development to market needs.

The NETL-RUA has matured over the past year by soliciting more input and feedback from its members including identification of research gaps and new thrusts that can be used for R&D planning.

The NETL-RUA draws resources from all its partners to provide the best available talent and capabilities to rapidly conduct focused, successful research projects.

Objectives:

1. Create and enable the *right* research teams to conduct the *right* research that effectively meets emerging national needs for science and technology.
2. Build R&D partnerships with the capability and expertise to be a force in the discovery, development, and deployment of next-generation technologies.
3. Discover and develop the technologies that will launch the next energy economy.

One way to describe the capabilities of the NETL-RUA is by its core competencies. The following three core competencies are what enable the NETL-RUA to develop and deploy energy technology for the sustainable production and utilization of fossil fuel resources:

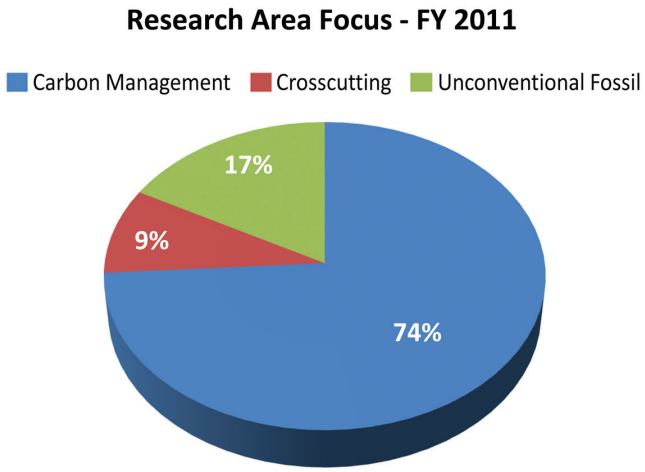
- Validated simulation-based science and engineering
- Materials discovery, characterization, development, and deployment
- Development and optimization of engineered systems

These competencies were applied to the research efforts that can be categorized into three key fossil energy areas:

1. Carbon Management
2. Cross-Cutting Research
3. Unconventional Fossil

The distribution of funding that was provided to projects in each of these three research categories in FY2011 is provided in the pie chart at right.

The portfolio of research efforts was managed through a set of 21 research teams comprising of researchers from NETL, the Alliance universities, and the URS site support contractor. Each of the teams identified in the table below was focused on a given energy grand challenge and worked collaboratively to address the research needs.



FY2011 NETL-RUA Research Teams

Competencies

1. Validated Simulation-Based Science and Engineering
2. Materials Discovery, Characterization, Development, and Deployment
3. Development and optimization of Engineered Systems

Research Area Focus	Carbon Management	Cross-Cutting	Unconventional Fossil Resources
Research Teams	▪ Advanced Combustion ▪ Advanced Gasification ▪ Carbon Capture ▪ CO_2 Utilization ▪ CO_2 Storage-Reservoir ▪ CO_2 Water-Rock Chemistry ▪ Energy Storage ▪ Environmental ▪ Fuels ▪ Fuel Cells ▪ Turbines ▪ Membranes ▪ Multi-Scale, Multi-scale Flow Fluid Flow ▪ Quantitative Risk ▪ Quantitative Monitoring, Verification & Accounting	▪ Advanced Simulation ▪ Sensors	▪ Extreme Drilling ▪ Hydrates ▪ Seal Integrity ▪ Unconventional Fossil – Shale Gas

Major FY2011 research accomplishments are summarized by core competencies in the proceeding pages.

Validated Simulation-based Science and Engineering

- AVESTAR™ Center Established

NETL-RUA established the AVESTAR Center with the deployment of two plant-wide IGCC dynamic simulators at locations at NETL and WVU's National Research Center for Coal and Energy, both in Morgantown, West Virginia. They are first-of-a-kind dynamic simulators and operator training systems (OTSs) for an IGCC power plant with 90% pre-combustion CO_2 capture and compression.

NETL-RUA is leveraging the AVESTAR Center to lead efforts to develop dynamic simulation and control technology for the safe, reliable, and efficient operation of pre-, post-, and oxy-combustion carbon capture processes for industrial applications.

NETL-RUA researchers integrate physical and chemical experimental research with computational sciences as the preferred method for understanding and developing technologies, advanced materials, and multi-scale energy systems at the molecular, device, and plant scales.

To further leverage the AVESTAR facilities and simulators, NETL and its NETL-RUA partners are pursuing an innovative R&D program in the areas of high-fidelity dynamic equipment reduced order modeling, advanced process control, sensor placement, and 3-D virtual plant simulation.

- C3M™ Software Licensed

The C3M software couples the kinetic rates for devolatilization, secondary tar cracking, and char gasification with NETL's multiphase CFD solver MFIX and leading commercial CFD solvers ANSYS-FLUENT and Barracuda.

The C3M graphical user interface provides easy access to the commercially available coal kinetic databases PC Coal Lab and FG-FVC, and the open-source devolatilization package CPD.

Near-term development of C3M will include soot oxidation and gasification and an interface for extracting kinetic rates from thermogravimetric analysis (TGA) data that is suitable for use in CFD modeling.

- First-of-a-kind Multiphase Flow Simulation Capability Developed

NETL-RUA researchers developed advanced capabilities for simulating multiphase flow. It is for the first time possible to simulate the multiphase flow behavior of gas-solid flows using millions of particles with parallelization of NETL's multiphase open-source CFD solver MFIX-DEM.

A discrete element method (DEM) provides an accurate description of granular flows with explicit accounting of particle-particle interaction.

The recent addition of heat and mass transfer to MFIX-DEM, which couples fluid flow with granular flow, enables accurate simulation of gas-solid flows that are encountered when using fossil fuel as a source of energy.

- CCSI Launched

NETL-RUA launched CCSI to accelerate the development of carbon capture technologies. CCSI will provide a simulation toolset consisting of a validated suite of models and simulation tools that enable the rapid development and deployment of new carbon capture technologies to technology developers and plant operators.

The project was launched in February 2011 after the plan was externally reviewed and accepted by a panel of eminent scientists and engineers from industry, academia, and national laboratories. The initial elements of the CCSI Toolset were successfully demonstrated at the September 2011 Industry Advisory Board Meeting.

- APECS wins R&D 100 Award

NETL's Advanced Process Engineering Co-simulator (APECS), Version 2.0, has been selected for a 2011 R&D 100 Award.

APECS v2.0 is a versatile, innovative, and powerful software toolkit for developing next-generation energy plants using advanced process and equipment co-simulation coupled with comprehensive design optimization.

Version 2.0 supports the recently released ANSYS-FLUENT® v13.0 computational fluid dynamics (CFD) software, including enhanced support for advanced combustion and dense multiphase-flow gasification applications. APECS v2.0 also allows the systematic generation of fast, accurate, CFD-based reduced order models (ROMs), including time-averaged ROMs based on transient CFD simulations, using a pioneering off-line ROM Builder.

The seamless and tight integration of the ROM Builder with the recently released ANSYS DesignXplorer™ v13.0 provides even more new ROM features that make it easier, faster, and less expensive for engineers to optimize existing and future plant designs with a high degree of confidence.

Materials Discovery, Characterization, Development and Deployment

- Discovery of Composite Material with Improved Capture Solvent Properties

Researchers at NETL performing theoretical studies on ionic liquids (ILs) confined within carbon nanotubes (CNT) have discovered the presence of nano-scale ordering, which has profound implications for the gas transport properties of the system.

The composite material exhibits higher sorption selectivity for CO_2 over H_2 than either the IL or the CNT, leading to improved capture solvent properties in the hybrid.

NETL-RUA is unique worldwide in that it has facilities for alloy development, melting, casting, fabrication, physical and chemical analyses and performance testing (wear, erosion, and various forms of corrosion).

- Photocatalytic Material Behavior Characterized for Direct CO_2 Conversion Application

  The NETL-RUA has recently developed and utilized a validated computational approach to accurately characterize the interaction of CO_2 with photo-catalytic materials. Specifically, the efforts have resulted in a basic understanding of the reaction pathway and the surface characteristics that need to be exploited for optimal reactivity and conversion in larger scale systems.

- MOFs Demonstrate Dynamic Carbon Capture

  The NETL-RUA has collaborated with the National Institute for Standards and Testing (NIST) to develop and demonstrate a novel CO_2 capture sorbent. Through complementary investigations including high-pressure surface science and laboratory reactor scale performance assessment, novel structurally dynamic metal organic frameworks have been shown to selectively absorb CO_2 from mixed gas streams containing N_2 and CH_4.

- Successful Cast of Superalloy for Ultra-Supercritical Steam Boiler and Turbine Applications

  The NETL-RUA, in collaboration with MetalTek and General Electric, is developing critical foundry parameters necessary to successfully cast Ni-based gamma prime strengthened superalloy that is traditionally wrought.

  A 300-lb step-block recently cast at MetalTek was developed using a process developed in the NETL-RUA Melting-Fabrication-Heat Treatment Laboratory and is currently being evaluated at General Electric and NETL to determine an optimal homogenization heat treatment for tailored microstructure.

- Robust Membrane Materials Analyzed for Pre-Combustion Capture

  The NETL-RUA has utilized computational approaches and experimental databases to construct thermodynamic-based corrosion stability diagrams for relevant hydrogen separation materials for use in pre-combustion conditions and environments.

  The analysis has been used to verify and understand the evolution of corrosion products on over 30 coupon samples that had been tested for over 1000 hours at the National Research Center for Coal and Energy (NRCCC) under "real" syngas conditions, and will be used to design new separation materials tailored for these harsh environments.

- Cathodes Identified for High Capacity Energy Storage Applications

  The NETL-RUA has identified a variety of novel cathode architectures that show potential for stationary energy storage applications, potentially increasing process efficiency and reducing the greenhouse gas footprint of fossil-based power production.

  Initial capacities of the $MgMnSiO_2$ and spinels ($MgMn_2O_2$) have been measured as high as 350mAh/g for the laboratory scale cathodes, exhibiting a greater than 300% increase in performance as compared to literature values for $MgMnSiO_2$.

NETL-RUA addresses energy security by conducting research that maximizes reliable use of domestic energy sources and infrastructure while minimizing the environmental impact of fossil fuel production and use.

Development and Optimization of Engineered Systems

- Improved Equations of State Better Predict Hydrocarbon Fluid Behavior Under Extreme Conditions

  Prediction of fluid behavior at high pressure and temperature (both in reservoir and wellbore environments) is critical for ensuring the safety of producing unconventional fossil resources in deep reservoirs. However, current physical models are tailored to less extreme conditions associated with conventional production.

  NETL-RUA researchers (in collaboration with Virginia Commonwealth University) are developing improved predictive relationships for fluids under these conditions by expanding experimental databases to include these extreme conditions (up to 500 °F and 35,000 psi).

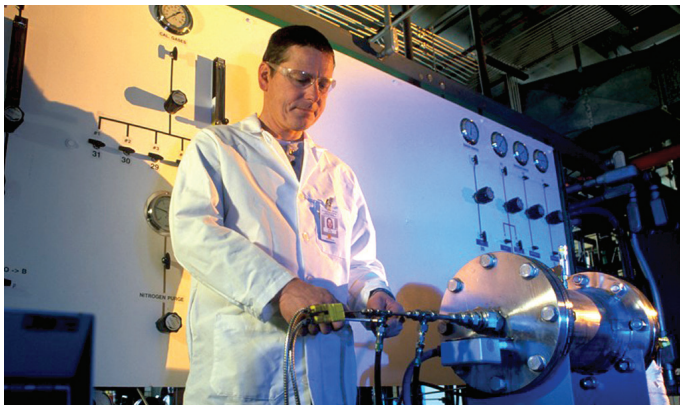
  Data on compounds studied to date have already helped identify improved equations for key physical parameters at these conditions.

- Chemical Self-Sealing Behavior Exhibited in Damaged Wellbore Cement

  Wellbore integrity is recognized as a key component of long-term CO_2 storage, and there has been concern that acidic carbonated brines might compromise this integrity by corroding the cements used in completions.

  NETL-RUA researchers (in collaboration with University of Texas, Austin) used a high-pressure, high-temperature experimental system to simulate the flow of carbonated brines along an imposed fracture in wellbore cement. The experiment provided evidence that, for some reactive-flow regimes, cement is dissolved in parts of the fracture but re-precipitated in other parts, thereby causing the flow path to seal over time.

  These experiments provide quantification and validation data needed for risk assessments that must predict the behavior of wellbores over long periods of time.



Hydrogen Separation – Synthesis, processing, fabrication, and performance evaluation of membranes.

- Public-Private Collaboration with Shale-Gas Producer Monitors Environmental Impacts

  NETL-RUA researchers spearheaded a public-private collaboration to document environmental baselines and changes resulting from shale-gas development.

  NETL-RUA researchers used an existing collaboration with a prominent shale-gas producer to broker the development of a field test site that will be used to monitor numerous environmental signals prior to and during development and production of gas from the Marcellus Shale.

  This study will document potential impacts attributable to shale-gas development relative to natural baselines. NETL-RUA researchers are also pursuing similar opportunities with other industrial partners.

- Improved Method for Estimating CO_2 Storage Potential

  NETL's Carbon Sequestration Atlas has proved to be an invaluable resource for a variety of stakeholders by providing regional and national estimates of storage potential.

  NETL-RUA researchers have revised the underpinning quantification methodology for the Atlas based on a rigorous statistical evaluation of parameters, allowing for improved estimates of CO_2 storage potential in future editions of the Atlas.

NETL-RUA researchers have also demonstrated that this rapid methodology compares well with a new, more complicated methodology under development by the United States Geological Survey (USGS).

NETL-RUA addresses energy security by conducting research that maximizes reliable use of domestic energy sources and infrastructure while minimizing the environmental impact of fossil fuel production and use.

- Isotopic Tracers Differentiate Sources of Groundwater Impacts

Development of the Marcellus Shale occurs in a region with a complex geology and a complex history of non-shale-gas resource development, both of which can impact groundwater chemistry. To differentiate potential impacts due to shale gas from other variations in groundwater chemistry, NETL-RUA researchers are investigating a variety of natural isotopes that are sensitive to different sources.

These chemical signals can be monitored using cutting-edge analytical facilities developed within the NETL-RUA, and early results from a field site have already demonstrated the ability to differentiate impacts due to mine drainage from potential impacts associated with shale-gas development.

- Methane Hydrate Reformation Phenomenon Confirmed

Laboratory experiments confirmed the predicted reformation of hydrate during methane-gas production from hydrate-bearing sand, a phenomenon that poses a potential impediment to continuous gas production from a reservoir.

However, the phenomenon has never been observed in the field. The NETL-RUA experiments provide confirmation for predictive codes and will enable the ability to elucidate the details of the reformation process and potential strategies to address it. The research was published in *Energy & Fuels* (2011, 25:1099–1110). (Yongkoo Seol and Evgeniy Myshakin)

- Dry CO_2 Sorbent Performance Tested & Validated for Carbon Capture

NETL's Carbon Capture Unit (C2U), a circulating fluidized bed reactor system that began operation in FY2011, is being used to validate the performance of dry sorbents in a complete process for carbon capture. Compared to conventional flue gas solvent CO_2 scrubbing systems, dry CO_2 sorbents can avoid the significant energy penalty connected with solvent-water vaporization.

Sorbent Materials Development – Sorbents have potential to reduce regeneration energy requirements compared to solvents, but they require new reactors and materials handling techniques.

Earlier in FY2011, NETL-RUA experimentally characterized the performance of CO_2 sorbents so that CCSI could develop a model for sorbent capture reactor systems. This is important because there is no prior guidance on how to develop dry sorbent systems to capture CO_2. The modeling results are being used to guide validating experiments in the NETL C2U.

- Chemical Looping Oxygen Carrier Performance Tested

NETL's Office of Research and Development (ORD) is investigating chemical looping as a relatively new approach for CO_2 capture from power plants or process heaters. Because chemical looping isolates CO_2 as an inherent part of the reaction process, there is no energy penalty associated with separating CO_2.

Experimental tests of several oxygen carriers for chemical looping were completed during FY11, and conditions/properties needed to avoid unwanted carbon deposition were determined. These data are important to an ongoing effort to both model and experimentally validate chemical looping.

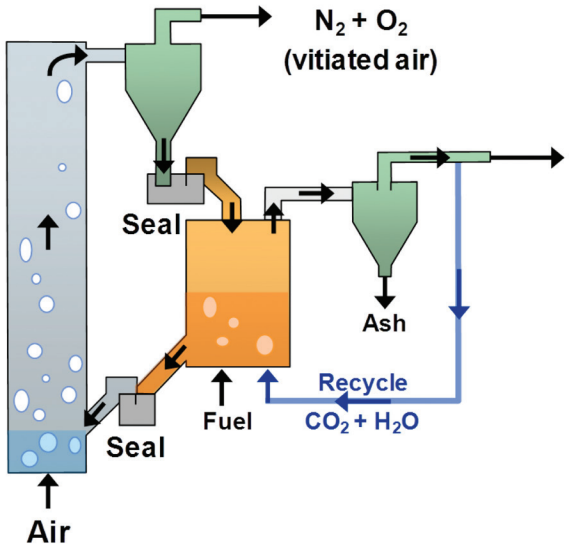
- New Instrument Measures Fuel Gas Composition in Real-time

The composition of fuel gas and other process gasses is important to successful operation of advanced energy systems.

Existing measurement technology is too slow or costly to provide useful data for process operation. For example, gas chromatography requires several minutes to characterize some gas streams, which is too long for most process control.

The analyzer uses fiber optics and Raman lightscattering to analyze the composition of gas streams, so the complete composition of most common process gas streams can be identified in less than one second with accuracy comparable to or better than that of existing approaches.

The packaged sensor will be tested by a commercial partner in FY2012.



Chemical looping process flow diagram illustrates isolation and recycle of CO_2.

Strategic Priority #2:

Increase Economic Impact

Develop and pursue new business opportunities and funding sources to grow the NETL-RUA research portfolio and capabilities, and leverage core competencies to a broader range of energy and environmental issues and a larger client base.

Growing the Research Portfolio

Objectives:

1. Expand NETL-RUA funding resources and research portfolio by successfully pursuing opportunities that leverage the core capabilities, expertise, and activities of the NETL-RUA.
2. Develop strategic partnerships with industry, institutions, other laboratories, and international entities as well as inter-agency in order to obtain access to additional resources.
3. Facilitate the identification, development, and implementation of unique research facilities that can serve as NETL-RUA signature resources

Leverage the Core Capabilities, Expertise, and Activities of the NETL-RUA

Response to Funding Opportunities

FY2011 NETL-RUA funding came almost exclusively from the DOE Office of Fossil Energy. However, during FY2011 the NETL-RUA pursued opportunities to diversify funding sources and provide for greater impact of its research capabilities. The NETL-RUA submitted approximately 20 proposals for additional funding for which the results of five were announced by the close of FY2011. The NETL-RUA won four of the five announced awards (80%), worth a total of $4.51 million.

The four joint NETL-RUA proposal efforts that were successful in gaining award funding were the following:

1. Role of Gas Hydrates during the Release of Well Fluids into the Deep Ocean (Lead: NETL)
2. Optimizing parameters for predicting the geochemical behavior and performance of discrete fracture networks in geothermal systems (Lead: NETL)
3. Nanocomposite Magnet Technology for High Frequency MW Scale Power Converters (Lead: CMU)
4. CFD Model Validation and Verification for High-Level Radioactive Tank Waste at Hanford (Lead: NETL)

NETL and the NETL-RUA responded to 51 solicitations from January to September 2011. The funding sources for those solicitations are represented by the pie chart below.

Research award announcements for the balance of NETL-RUA jointly-pursued proposals (with a combined value of over $23 million) were pending at the conclusion of FY2011.

The proposal work done to date has been noteworthy, but efforts to obtain additional research work through newly developed collaborations are being planned.

Strengthening and developing relationships with new university professors, NETL researchers and industrial partners will create new synergies and provide increased opportunities for proposal development and lay the groundwork for future funding award success.

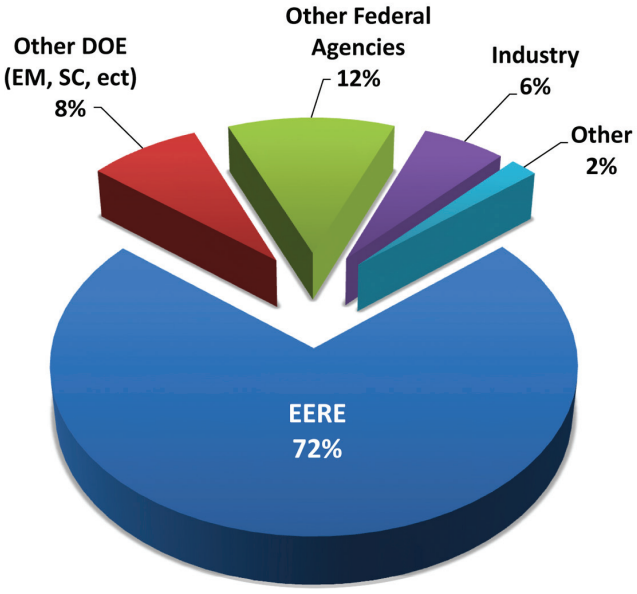
Distribution of the NETL-RUA proposals by the lead organization is presented in the chart below.

Strategic Growth

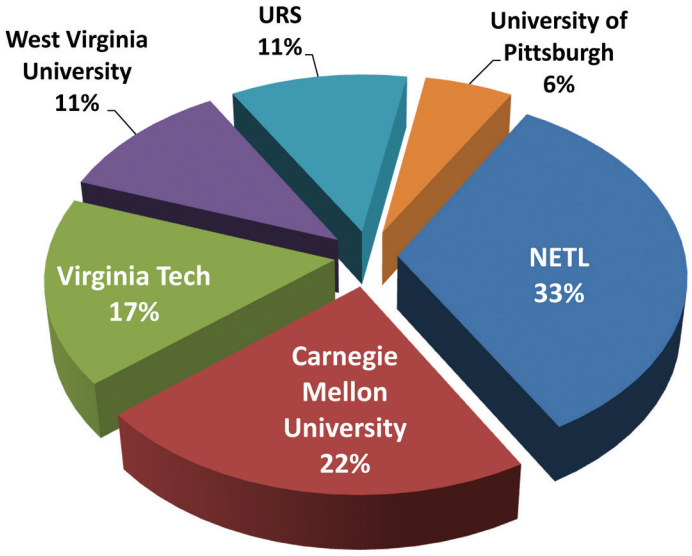
NETL-RUA spearheaded a strategic push to grow the research portfolio with the introduction of Strategic Growth Areas (SGAs) and associated activities that promoted all of the NETL-RUA's strategic goals. This new approach to growth was in large part a response to the recognition that the pathway to greater NETL-RUA effectiveness, measured in market acceptance of beneficial new technologies, is to develop energy solutions in conjunction with industry partners. Another was an acknowledgement that continued pressure on the DOE Fossil Energy budget is expected to limit the available funding from the Office of Fossil Energy for NETL-RUA research in coming years.

In May 2011, the NETL-RUA Executive Committee decided to push the development of new research, partnerships, and funding through a workshop focused on six areas of energy infrastructure needs in which the NETL-RUA has the potential make significant and highly valued contributions. Teams consisting of representatives from all NETL-RUA organizations met for two days to characterize these areas and plan a strategic approach for each.

Funding Opportunity Source



Proposals by Leading Organization



The six SGAs investigated included:

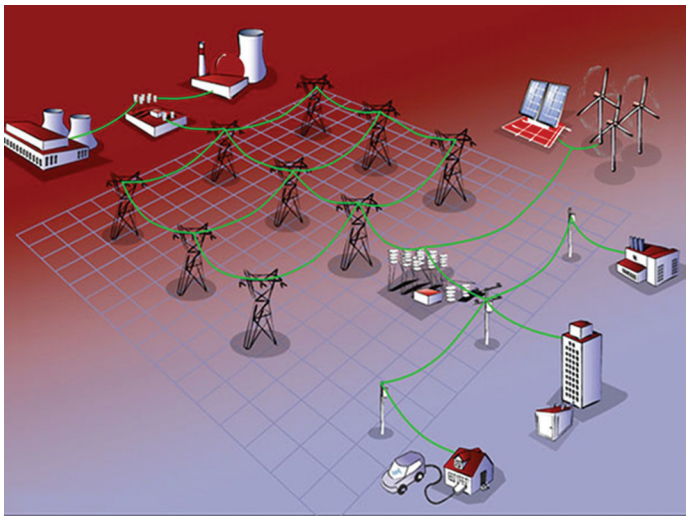
- Power Grid Technologies
- Rare Earths and Critical Materials
- Shale Gas
- Advanced Materials
- Energy Storage/Batteries
- Energy/Water Nexus

On the strength of the resulting plans, two SGAs—Power Grid Technologies and Rare Earths/Critical Materials—were selected for joint investment by the NETL-RUA Executive Committee. The other SGA teams were asked to focus and strengthen their proposed plans for research, partnership, and growth and given the opportunity to present revised plans to the Executive Committee when they could make a more compelling case for seed investment. It is anticipated that the Shale Gas and Advanced Materials SGAs will rework their plans for eventual presentation to NETL-RUA's Executive Committee for additional support. Parts of Energy Storage/Batteries and Energy/Water Nexus were absorbed into the Grid Technologies and Shale Gas efforts, respectively, and are not expected to develop into full SGA efforts in the near term.

Power Grid Technologies

The Grid Technologies SGA was selected by the Executive Committee as being well positioned in what is forecast to be a very large market for upgrading U.S. transmission and distribution systems and as an enabling technology for transitioning to a sustainable energy economy.

The Grid Team has made great strides in developing the formal NETL-RUA Grid effort, capitalizing on broad participation from all its members. Strengths within the effort include it not being dependent on winning a major competition (e.g., a funded hub) for sustainable growth; it builds upon a proven growth model; and it is based on a strong strategy for technology development and market approach that includes regional support, students, and alignment of NETL-RUA interests and capabilities.



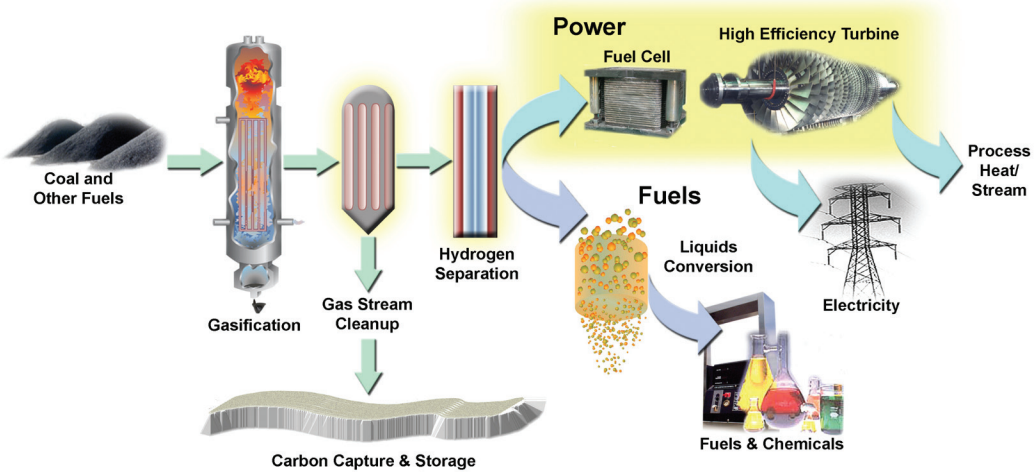
Replacing the old outdated power grid with new innovative equipment and installing computer controls and software will guard against power outages and provide higher reliability.

The plan for this area is focused on developing a Grid Technologies Collaborative (GTC) consisting of researchers from NETL-RUA and industry to execute a comprehensive program of fundamental research on power electronics technologies for transmission and distribution system applications; technology development, simulation, testing, and commercialization; and professional training for the advanced grid technologies sector.

The NETL-RUA Grid Team plans for a first-year focus on consolidating capabilities across partner institutions and building a market and brand recognition for innovative R&D, technology integration and training services within the initiative.

Plans also include support from the Executive Committee to hire a business development and marketing expert to develop material, build relationships with industry, and attend key meetings and symposia advertising the capabilities of the GTC.

A more comprehensive business plan and resource estimate will be developed by the Grid Team in 2012 and presented to the Executive Committee.



Advanced materials are essential to coal fuel and advanced power generation systems.

Critical Materials

The NETL-RUA Executive Committee determined that the Critical Materials Research Alliance (CMRA) Team should develop a business plan in preparation for potential upcoming funding opportunities.

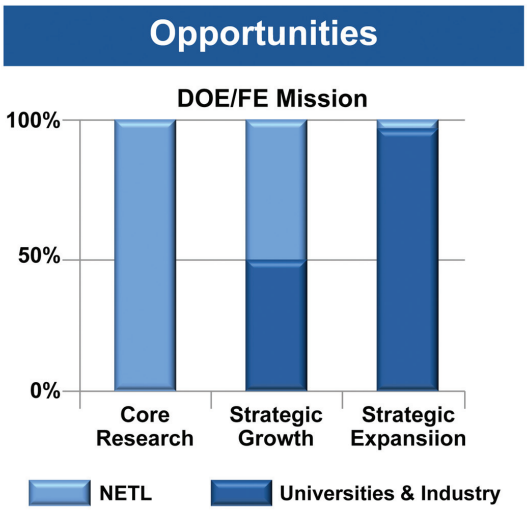
NETL-RUA's capabilities in mining and materials research are well-suited to address research focused on uncovering additional and cost-effective sources of rare earths and critical materials, as well as reducing the need for or replacement with lower cost or more readily available materials. The business development approach is focused on successfully competing for a potential DOE energy hub in 2012. A unique team has been assembled that includes a major materials industry partner and heavy participation by each NETL-RUA university partner.

The business plan technical approach has been to assess each area of potential research need against collaboration capabilities. Where gaps were identified, additional partners, including academic partners, are being added to the team. The CMRA will present their plans for the potential hub development to the Executive Committee in 2012.

Other Growth Opportunities

The Strategic Growth Areas represent only one approach to an expanded NETL-RUA role in the regional and national energy economy.

NETL-RUA researchers and teams are invited to submit proposals to funding organizations for research that may fall outside the SGA's scope or the DOE/Fossil Energy mission. The laboratory may still participate in such research, but seed funding and the leading role would have to be taken by a non-federal member organization.



As opportunities extend further beyond NETL's core FE mission, its NETL-RUA partners will have to take the lead.

Develop Strategic Partnerships

Industry

The NETL-RUA has sought out industry partnerships in an effort to better understand industry market and technological needs, meet governmental regulatory goals, and streamline technology application and commercialization.

Several initiatives which include NRAP, CCSI, and the SGA initiatives have leveraged strengths within industry, universities, and federal laboratories to provide specific problem-focused solutions to emerging energy technology challenges. These partnerships expand the power and capabilities of the NETL-RUA, and develop solutions that meet industry needs. Partners include:

Industrial

ADA Environmental Solutions
Alstom Power
Ameren
Babcock Power
Babcock & Wilcox
Chevron
Electric Power Research Institute
Eastman
Fluor
General Electric
Ramgen Power Systems
Southern Company
URS

Academic

CMU
Penn State
Princeton University
Pitt
Virginia Tech
WVU

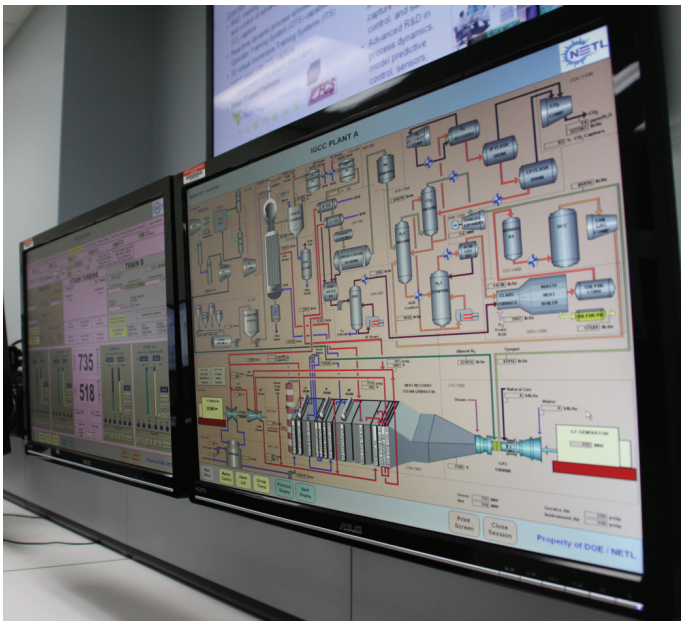
National Labs

NETL
Lawrence Berkeley National Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
Pacific Northwest National Laboratory

University Energy Partnership (UEP)

A relationship between the University Energy Partnership (UEP) and the NETL-RUA is currently being developed. The UEP comprises the same universities that are members of the NETL-RUA (CMU, Penn State, Pitt, Virginia Tech, and WVU), but is focused on initiatives that directly relate to its five university members.

The UEP is a non-profit university consortium chartered to enable its university partners to collaborate effectively toward their shared goal of national leadership in advancing energy options for NETL and the region.



Avestar Simulator power plant process flow diagram is used to virtually control operations.

In particular, the partnership will promote the growth and strengthen the reputation of:

- Energy-related research and education within its partner universities
- Onsite research at NETL
- The regional energy innovation economy (including technology commercialization, education, and workforce development at all levels) and will expand economic opportunity within an export-focused industry cluster as well as its local supply chain.

The NETL-RUA seeks to partner with the UEP and, when interests align, draw on its capabilities. The relationship has already yielded collaboration within the Grid Strategic Growth Area project.

The UEP has forwarded funds for a business development professional to aid in developing the NETL-RUA's Grid SGA.

Additional potential areas of collaboration that meet the NETL-RUA's commercialization objective exist as well as the opportunity to deploy new technologies stemming from its activities.

The UEP's relationship with the region's commercial energy sector and its focus on serving as the basis for regional economic development and nationwide job creation provides a strong foundation for continued collaboration.

NETL-RUA Signature Resources

AVESTAR™ Center, NETL-Morgantown and WVU

The NETL has collaborated with industry and university partners to establish the world-class AVESTAR Center dedicated to the operation and control of advanced energy plants with carbon capture.

Facilities and Features:

- Two training and research locations in Morgantown, West Virginia
- High-fidelity, real-time dynamic simulators
- IGCC power plant with CO_2 capture
- Full-scope OTS in a state-of-the-art control room environment
- Immersive training systems (ITS) in a realistic 3-D virtual plant environment

The AVESTAR Center offers a collaborative R&D program and comprehensive hands-on training built around a portfolio of non-proprietary, high-fidelity, real-time dynamic simulators. The simulators provide OTS capabilities for normal and faulted operations as well as plant start-up and shutdown. The benefits of high-fidelity ITSs include more realistic training scenarios, improved communication and collaboration among work crews, off-line evaluations of procedures, and training for safety-critical tasks and rare abnormal situations.

By providing comprehensive virtual energy plant OTS and ITS solutions, the AVESTAR Center will develop a workforce well-prepared to operate and control commercial-scale power plants with carbon capture.

The AVESTAR Center, located at NETL in Morgantown, West Virginia and at WVU's National Research Center for Coal and Energy, is operated with support from the URS Corporation and the NETL-RUA.

Immersive 3-D virtual reality adds a dimension of realism to training scenarios.

Simulation Based Engineering User Center

On September 16, 2010, Department of Energy Secretary Steven Chu announced the creation of the Simulation-based Engineering User Center (SBEUC), located at NETL. The center will facilitate collaborative computational research for energy applications. Funded with $20 million from the American Recovery and Reinvestment Act, the SBEUC will be used primarily for developing and deploying the simulation tools developed under CCSI.

The SBEUC will accelerate the research and development of CCS technologies and support the Administration's goal to overcome the barriers to widespread, cost-effective deployment of CCS within 10 years.

The SBEUC will provide resources to national laboratories to advance the following areas:

- Development of a high performance computing user center as a platform for utilization of the advanced simulation tools.
- Accelerating the deployment of industrial carbon capture technology through enhanced ability to predict industrial-scale performance.

A high-performance computer will allow researchers to simulate phenomena that are difficult or impossible to investigate experimentally. The results from simulations will become accessible through user centers that provide advanced visualization capabilities and foster collaboration among researchers.

> ***"This center (SBEUC) will not only help fight climate change, it will create new jobs and position the United States as a leader in carbon capture and storage technologies for years to come."***
>
> —Steven Chu, DOE Secretary of Energy

Advanced Turbine Laboratory at Penn State

As an NETL-RUA partner, Penn State will help lead collaborative efforts with UTC's Pratt & Whitney Division to design and construct a new world-class test facility that will significantly enhance turbine research. Its primary focus will be new cooling improvement strategies for the turbine rotating blade platform that will increase turbine efficiencies.

The Advanced Turbine Laboratory, projected for completion in FY2013, will be the most advanced stationary gas turbine testing facility in the United States and worldwide. The new laboratory will provide researchers the opportunity to model and perform laboratory testing on the next generation of gas turbine engines for improved fuel efficiency.

According to Dr. Karen Thole, professor and head of mechanical and nuclear engineering at Penn State, this research has the potential to reduce crude oil usage by about 25 million barrels per year and associated greenhouse gas emissions by 10 million metric tons per year.

NETL-RUA Isotope Analysis Facility at University of Pittsburgh

A new NETL-RUA isotope analysis facility at Pitt will enhance research in geology related to energy exploration and environmental assessment through a state-of-the-art technology multi-collector - inductively coupled plasma - mass spectrometer (MC-ICP-MS), a laser ablation workstation, and a desolvating system. The primary advantage of MC-ICP-MS is its ability to measure isotope ratios for a broad range of elements, including those with high ionization potential that are difficult to analyze by other techniques.

Diligent NETL-RUA teamwork and planning led to the installation of the $750,000 MC-ICP-MS at the Pitt laboratory, where numerous university and NETL researchers have been running samples. The MC-ICP-MS technique has been successfully applied to a wide variety of topics including geo-chronology/thermo-chronology, fluid/rock interaction, and biogeochemistry and adds a new level of sophistication to NETL-RUA carbon capture and storage research.

The tool, with maturity, will become increasingly important for quantifying, assessing, and monitoring environmental systems, in addition to current geological applications. It will find widespread applications and acceptance in other disciplines, such as environmental science, biology, biochemistry, ecology, and archaeology.

Chemical Looping Reactor Test Facility at NETL

Chemical looping technology will be the predominant technology to be developed by the NETL-RUA for industrial carbon capture. Chemical looping is part of the Industrial Carbon Management Initiative (ICMI) which will leverage computational and experimental methods, ranging from materials design through techno-economic process development, to evaluate and develop carbon management strategies for industrial sources other than fossil energy electric power generating plants.

This effort will evaluate significant industrial sources of CO_2 emissions, assess promising technology options for cost-effective CO_2 reduction, develop and validate simulation models that can accelerate technology deployment, and develop appropriate sequestration and reuse methods for the captured CO_2.

The objectives of the project are to:

- Evaluate significant industrial sources of CO_2 emissions and assess promising technology options for cost-effective CO_2 reduction
- Develop simulation models that will be powerful tools to accelerate technology deployment, minimize deployment cost and risk, and identify gaps for further targeted research
- Design, install, and operate a chemical looping reactor (CLR) facility for industrial natural gas applications to develop sensors and diagnostics, develop improved materials, and obtain critical thermal science and engineering data to calibrate simulation models
- Develop appropriate sequestration and reuse options for the captured CO_2
- Conduct a techno-economic analysis to project costs and benefits of deploying technology developed in this initiative

Literature searches were begun on coal and methane kinetics during FY2011. The initial engineering and design work was completed and procurement began on numerous items such as vent line filters, secondary heaters, and instruments. Structural work advanced considerably.

Strategic Priority #3:

Accelerate Commercial Deployment

Facilitate the management, dissemination, and commercialization of the intellectual assets created through the NETL-RUA by leveraging its combined knowledge, experience, networks, and best practices to support energy innovation and entrepreneurship to stimulate economic growth.

Promote and Facilitate Conversion of Intellectual Assets into New Products, Processes, and Jobs

The Technology Transfer Committee—the focus of which is the management, dissemination, and commercialization of the intellectual assets created through the NETL-RUA—has leveraged the combined knowledge, experience, networks, and best practices of the NETL-RUA to support energy innovation and entrepreneurship.

Agreement Templates and Agreement Activities: The Committee is developing standard templates for intellectual property agreements and standard contract language in preparation for new business opportunities that may occur both external to and within NETL's current RES contract with URS and the universities.

The Technology Transfer Committee has undertaken several agreement initiatives dedicated to NETL-RUA research and operational processes that will increase its efficiencies within the NETL-RUA. Through proactively outlining and defining agreement parameters, the Technology Transfer Committee anticipates increased efficiencies in agreement execution and partnership development turnaround. Several of the projects under development include boilerplate language for Cooperative Research and Development Agreements (CRADAs), sponsored research agreements, Inter-Institutional Agreements (IIAs), and standard agreements for non-disclosure (NDAs) and memoranda of understanding (MOUs).

Objectives:

1. Promote, facilitate, and forge partnerships to convert intellectual assets into new products, processes, and jobs.
2. Share best practices of the NETL-RUA organization members to aid in the development of processes and agreements that advance the technology transfer mission.
3. Identify potential intellectual assets resulting from NETL-RUA research projects and optimize their value.

Share Best Practices to Improve NETL-RUA Technology Transfer

The NETL-RUA has utilized best practices generated from members' agreement templates in creating drafts for NETL-RUA operating agreements. Members' experience in executing research agreements and developing consortia dedicated to pursuing research initiatives has been critical in structuring an NETL-RUA agreement that meets member requirements, as well as considers industry's need for rapid transactions and research cycles.

Additional best practice efforts include member institutions presenting successful technology transfer practices for consideration by the NETL-RUA and individual members. In FY11, the NETL-RUA Technology Transfer Committee discussed best practices that focused on improving the technology transfer capabilities of member universities for the betterment of the NETL-RUA and each member institution. The best practices reviewed included CMU's standard technology spin-off practice, which included Terms, Templates, Misconceptions, and Philosophy; Penn State's development of a Technology Portfolio Valuation Process designed to calculate the monetary value of its intellectual property portfolio; and one of Virginia Tech's experimental best practices, which is driven by industry need to capitalize on a technology-pull model of research and development for technology transfer purposes rather than the traditional technology transfer model of technology push. Efforts are underway to leverage this expertise to provide the most effective execution of NETL-RUA technology transfer activities.

Identify and optimize intellectual assets from NETL-RUA research

There were several specific NETL-RUA accomplishments within the intellectual property domain, including 17 patent disclosures and the filing of three patent applications. An inclusive look at the global NETL Intellectual Property Statistics for FY2010 and FY2011 include:

NETL FY2010 and FY2011 Intellectual Property Statistics

Intellectual Property Management	FY2010	FY2011
Inventions Disclosed	30	17
Total Inventions Reviewed	13	20
Provisional Patent Applications	4	3
Non-Provisional Applications	12	9
All Patent Applications	16	12
Patents Issued	6	4

Pyrochem Catalyst Corporation

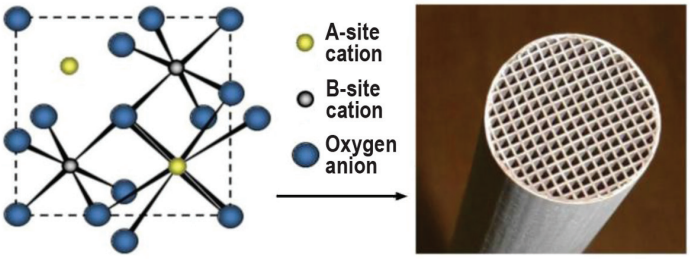
The lab's first start-up company was created as a result of the development by an NETL-RUA-led team of a new catalyst that converts hydrocarbon fuels to synthesis gas. Pyrochem Catalyst Corporation was established with the help of Pittsburgh's Innovation Works and obtained an exclusive license to the catalyst and a related NETL technology. The catalyst development team, which includes David Berry, Dushyant Shekhawat, Daniel Haynes (all NETL), Mark Smith (URS), and Jerry Spivey (LSU), recently received US Patent 8,133,463 on the pyrochlore-type catalyst.

A key potential benefit of this catalyst could be to enable the use of solid oxide fuel cells (SOFCs) for heavy truck idling. Professional truck drivers are mandated to rest for 10 hours after every 11 hours of driving. However, a power source is needed during these rest periods to provide heating, ventilation, and air conditioning to the cabin where they sleep and to power other electrical devices. Currently the

2.2 million diesel trucks that haul goods across the U.S. produce an estimated 11 million tons of carbon dioxide, 200,000 tons of nitric oxide, and 5,000 tons of particulate matter annually while idling, wasting more than 1 billion gallons of fuel. Auxiliary power units that incorporate SOFCs would allow drivers to obtain power from a reliable source while eliminating significant pollutant discharge, and could lead to use of similar units in large-scale power plants.

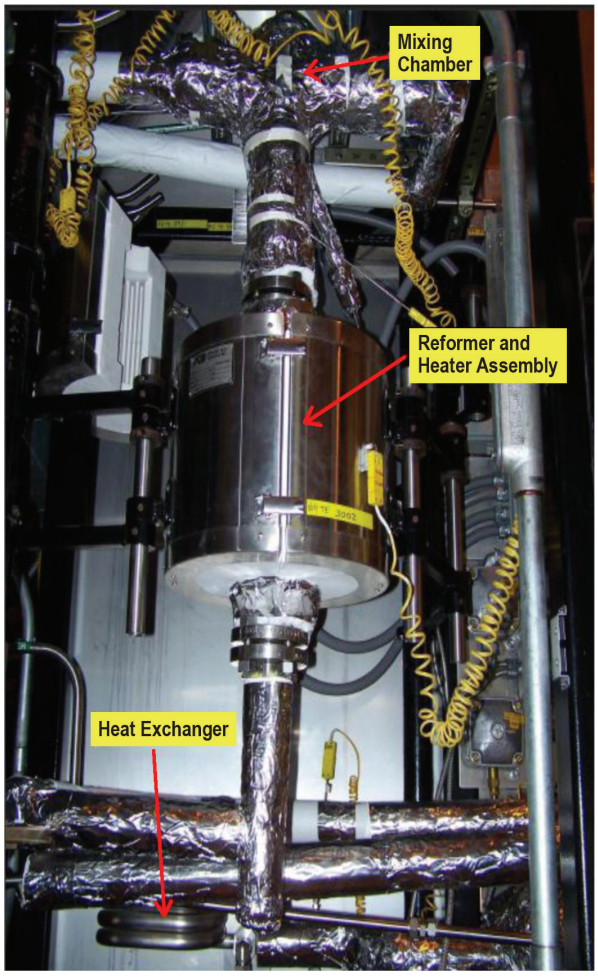
SOFCs are high-efficiency electrochemical devices that use hydrogen and oxygen to produce electricity. The hydrogen can be produced by converting fuels into synthesis gas, or syngas, a mixture of hydrogen and carbon monoxide, in a process called reforming. Syngas is currently generated from simple hydrocarbon fuels such as methane with the use of a catalyst. However, the sulfur and aromatic species in heavier, more complex fuels such as diesel pose a challenge because these components deactivate (or poison) conventional catalysts. Therefore, the development of an economical catalyst that can reform diesel and coal-based fuels into hydrogen-rich syngas is critical for this application.

A catalyst is prepared with the desired formulation and coated onto a monolithic structure.



Catalyst (above left) and coating on monolithic structure (above right).

This represents a commercially usable product for reforming applications. Once prepared, the structure is loaded into the reactor, commonly designated as the Fuel Processing Unit (FPU), located at NETL in Morgantown, West Virginia, where a number of reforming demonstrations have been conducted proving the commercial viability of the catalyst. The catalyst system has been used to reform a variety of fuels using different reforming modes. Numerous test runs have been performed using diesel and biodiesel, and the syngas stream was fed directly into an operating SOFC for production of electricity.



Reactor (Fuel Processing Unit).

Harbison-Walker Refractories Company: AUREX™ 95P

Developed by scientists at NETL and licensed to Harbison-Walker Refractories Company, AUREX 95P is the most significant improvement in gasifier refractories in over 25 years. It is now the material of choice for high-wear areas of advanced, high-temperature gasifiers. Its widespread use is accelerating gasification as a clean, efficient means of producing electric power and other products.

C3M™

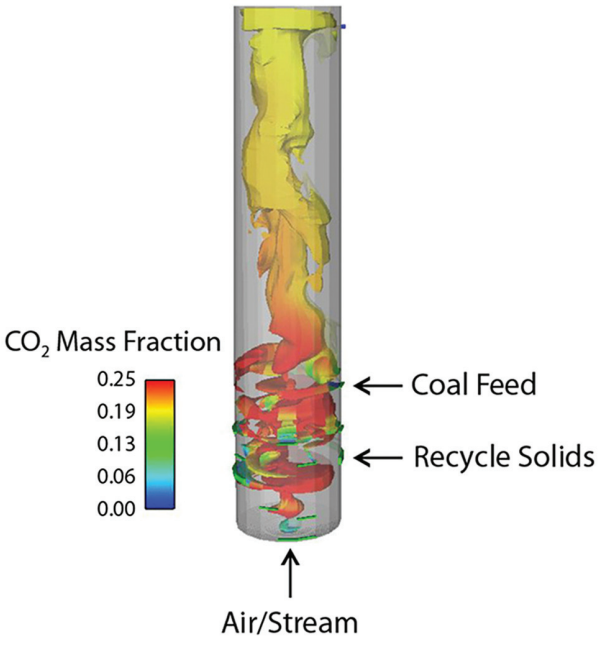
NETL has developed a software platform entitled C3M that is used to access a variety of kinetic processes and reaction mechanisms typically found in coal gasification, gas clean-up, and carbon capture processes. This unique software provides the user with the ability to conduct virtual kinetic experiments using leading kinetic packages and available experimental data to evaluate kinetic predictions as a function of fuel and sorbent type and/or operating conditions.

An international patent (Patent Cooperation Treaty) application was filed in June 2008. NETL is seeking non-exclusive licensing partners interested in implementing this software into their current systems and/or marketing it to industry.

The coal gasification industry is now at the forefront of a worldwide clean energy initiative. Industry experts agree that the markets for advanced technologies for gasification, gas clean-up and carbon capture are growing, with worldwide gasification capacity projected to increase along with stringent regulations for trace contaminant removal and aggressive targets for CO_2 capture.

Designing advanced gasification processes and devices requires an understanding of the physical transformations that fuel and sorbent particles undergo when exposed to hot, multiphase environments and the chemical reactions responsible for conversion of the solid material to gaseous species. The mechanisms responsible for a sorbent particle to remove pollutants from a gas stream must also be realized.

C3M augments existing computational fluid dynamic (CFD) software by helping researchers to model the complex interactions between gas and solid phases in a reacting environment. This software, coupled with a multiphase CFD model, allows a modeler to choose a kinetic process of interest (e.g., pyrolysis, gasification, sorbent based CO_2 capture, etc.) and evaluate it as a function of fuel and/or operating conditions.



A virtual kinetic experiment using C3M™.

Strategic Priority #4:

Prepare Tomorrow's Energy Leaders

Create a culture of energy leadership through promotion of education and entrepreneurship.

Creating Energy Leaders

There is an increasingly critical need for multi-stakeholder partnerships to provide knowledge, expertise, mentoring, and financial support to educate the next generation of energy leaders. NETL-RUA, through its research and educational programs, is poised to mentor young professionals to prepare them to perform innovative research and transfer new technologies to the marketplace.

Students participated on projects that totaled 41% of the FY2011 NETL-RUA research budget. In addition, 61 students obtained advanced degrees during 2010–2011 while working on NETL-RUA funded research efforts. Over 100 students, which includes undergraduates, were involved in NETL-RUA research in each of the past two years.

Objectives:

1. Establish collaborative energy education programs within the NETL-RUA using the research as a springboard.
2. Facilitate the exchange of personnel among NETL-RUA organizations.

		2010	2011
NETL-RUA Student Researchers		107	133
Advanced Degrees Conferred	**PhD**	20	20
	Masters	13	8

NETL-RUA partnerships encourage future generations to maintain U.S. leadership in the energy industry. From left, Scott Klara (NETL), Congjun Wang (URS), and Jonathan Lekse and Kristi Kauffman (NETL Student Interns).

Spotlight on Student Achievements

NETL-RUA graduate student, Elizabeth Chapman.

NETL-RUA grad student, Elizabeth Chapman successfully defended her Ph.D. dissertation at the University of Pittsburgh on November 21, 2011.

Her thesis, titled "Fossil Fuel Related Water-Rock Interaction in the Appalachian Basin, Pennsylvania and New York: A Geochemical Strontium Isotope Investigation," examined the use of isotopic ratios to fingerprint geologic fluids of interest in the Marcellus gas production area.

Chapman worked with University of Pittsburgh Professor Rosemary Capo on the Geochemical Tracers project as part of NETL-RUA's QMVA Research Team and contributed five posters and two podium papers, and is the primary author on a recently submitted journal article.

The NETL-RUA encourages multi-organizational thesis committees to provide the best experts for the research review. As an example of this, Dr. Harry Edenborn of NETL's Geosciences Division represented NETL on her thesis committee.

Collaborative Energy Education Programs

AVESTAR™ Center

In FY2011 NETL collaborated with industry and university experts to launch the world-class AVESTAR Center located at NETL and WVU.

An open house and CO_2 capture simulator-based training session was held during the DOE's multi-lab CCSI semi-annual review meeting.

The AVESTAR Center provides NETL-RUA with the opportunity to offer comprehensive training for operators, engineers, and managers; collaborate with energy experts on advanced research initiatives; enhance engineering education in process dynamics and control; and accelerate custom development of plant-specific simulators.

The AVESTAR Center hosted its first industry training course that provided participants with practical hands-on IGCC dynamic simulator training, including plant startup, shutdown, and power demand load following. Under the auspices of the NETL-RUA, chemical engineering professors at WVU are leveraging the IGCC dynamic simulator in undergraduate process design and control courses.

The AVESTAR Center has provided Power Plant Gasification training and demonstrations to ten individuals from industry and 40 NETL employees.

Operator training simulator for IGCC power plant with CO_2 capture.

Personnel Exchange

Researchers regularly access the NETL campus locations. Those researchers that visit on a regular basis to perform research and attend meetings are picture badged for access.

During FY2011, a total of 58 faculty members were badged for access to NETL (30 for NETL-Pittsburgh and 28 for NETL-Morgantown). This includes all Consortium Area Leads, Principal Investigators, Co-Principal Investigators and faculty.

In addition, a total of 38 others are picture badged for access to NETL (22 for NETL-Pittsburgh and 16 for NETL-Morgantown). This includes all graduate students, undergraduate students, post-docs and other researchers.

NETL researchers have also served as adjunct faculty for a number of member university courses. NETL researchers have been encouraged to participate as faculty and presenters within the NETL-RUA in an effort to increase reciprocal researcher relationships and provide students with access to subject matter experts.

A total of 45,120 hours of university faculty research were completed onsite at NETL in 2011.

Through the collaborative efforts of NETL researchers and university faculty, students are engaged in research and educational programs that prepare them to solve tomorrow's energy challenges.

Outreach and Impact

Increase the visibility and impact of NETL-RUA R&D as evidenced by contributions that affect a broad range of energy-related issues and through outside recognition for exceptional research efforts.

Advancing the Impact of NETL-RUA Research

External Outreach

Secretary Chu tour of the facilities for the 100 year celebration: Secretary of Energy Dr. Steven Chu and U.S. Senator Jay Rockefeller (WV) toured facilities at NETL in celebration of 100 years of NETL-sponsored RD&D programs.

Century of Science Presentation: The NETL-RUA was highlighted when NETL launched its second century of scientific advancement with an event at Pittsburgh's Carnegie Science Center on October 13, 2010.

During the event, NETL Director Dr. Anthony Cugini spoke about the benefits of the NETL-RUA partnership and the importance of marshaling a wide range of complementary skills, facilities, and ideas to solve the nation's energy challenges quickly and effectively. He also stated that the collaborative efforts of the NETL-RUA will produce results superior to those that individual organizations can achieve by acting alone.

Objectives:

1. Inform a diverse audience of the mission, importance, impacts, and successes of the NETL-RUA
2. Facilitate communication and sharing of information among NETL-RUA membership
3. Develop tools and materials that will assist NETL-RUA membership in championing the NETL-RUA

NETL Director Anthony Cugini welcomes guests to a Century of Science.

External NETL-RUA Website.

NETL-RUA External Website: An external facing website was developed during FY2011 for the NETL-RUA and is hosted on the NETL website. The website presents the integrated program team and the member universities as well as the NETL-RUA history and mission along with a link to the posted fact sheet. News and events, contact information, and a member's only area are also integrated into the website.

Various datasets are also available on DOE's website.

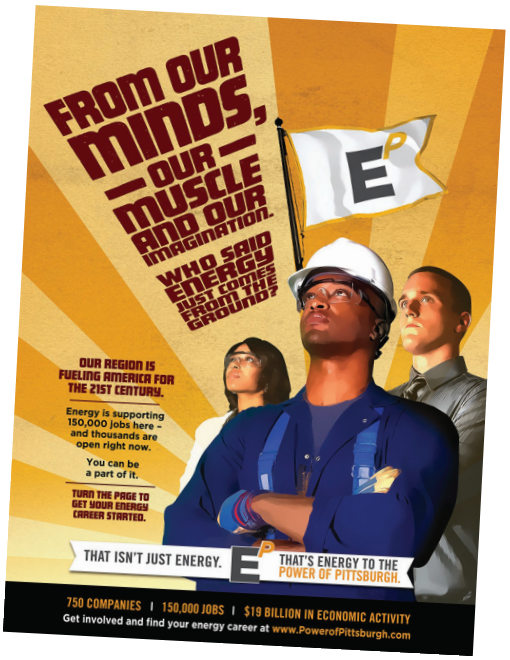
NETL-RUA Public Factsheet: NETL-RUA posted a fact sheet resource on the NETL website during FY2011 that presented an overview and the objectives of the NETL-RUA program. The fact sheet also provides contact information for the program participants.

Media Outreach

Televised Interview on WPXI-TV: Featuring Julianne Klara of DOE/NETL, Rich McCullough of CMU, and Gregory Reed of Pitt, on July 11, 2010. The interview was hosted by Bill Flanagan of the *Our Region's Business Program*, who moderated a discussion on regional energy opportunities through the NETL-RUA Program.

Newspaper Article: The *Pittsburgh Business Times* featured an article on October 29, 2010 entitled "National Energy Technology Lab will unite Pitt, CMU, others in research work."

Regional Promotional Campaign: Allegheny Conference leads "an initiative of nearly 100 companies, universities, government agencies, and non-profits dedicated to making the Greater Pittsburgh region the leader in American energy in the 21st century." The NETL-RUA, among several specific members, was featured in the conference's ad campaign E^P, which stands for *Energy to the Power of Pittsburgh*.



Energy to the Power of Pittsburgh Newspaper Advertisement.

Publishing Research Results: Publication counts can be viewed as a measure of research productivity. In FY2011, the NETL-RUA published nearly 200 peer reviewed papers, most of them jointly authored, describing the work performed under the auspices of NETL-RUA research teams. These papers are listed in Appendix C.

The table below illustrates the total number of peer-reviewed journal articles that researchers affiliated with the NETL-RUA published throughout 2011. These counts include all research efforts, not only those sponsored by the NETL-RUA. Compared to the nearly 200 publications for NETL-RUA-sponsored projects, this difference (200 versus 711) represents the potential research capability that could be tapped for NETL-RUA growth.

Citation indices provide a standard measure of research impact as they count the number of times a paper is cited rather than how many papers are published. The data in this table reveal that in FY2011, there were nearly 2,800 citations of publications by researchers affiliated with the NETL-RUA; citations of posters, presentations and other forms of publication bring that count to over 3,000. These data are one indication of the horsepower that the NETL-RUA can bring to improving the use of fossil-energy resources and developing the technological platform for this century's energy technology transition.

Internal Communication

NETL-RUA Members Only SharePoint Site (MOSS): This site went live in FY2011 and is available to all members of the NETL-RUA. It serves as both an information portal and workspace for teams and committees to share documents and collaborate. NETL-RUA research teams were given access to the MOSS to provide them with a collaborative work environment with controlled access.

NETL-RUA Spring Meeting: The event unveiled the NETL-RUA vision and expectations and presented the FY2011 collaborative research portfolio and FY2012 plans, including program status and committee updates.

The NETL-RUA spring meeting was well attended with more than 233 attendees, and included presentations on the NETL-RUA vision and expectations; NETL-RUA program status; FY2011 and FY2012 collaborative research planning; committee updates; contract requirements, issues, and expectations; concurrent research team and committee meetings; a presentation on "The Bell-Labs Model for Collaboration"; and networking sessions.

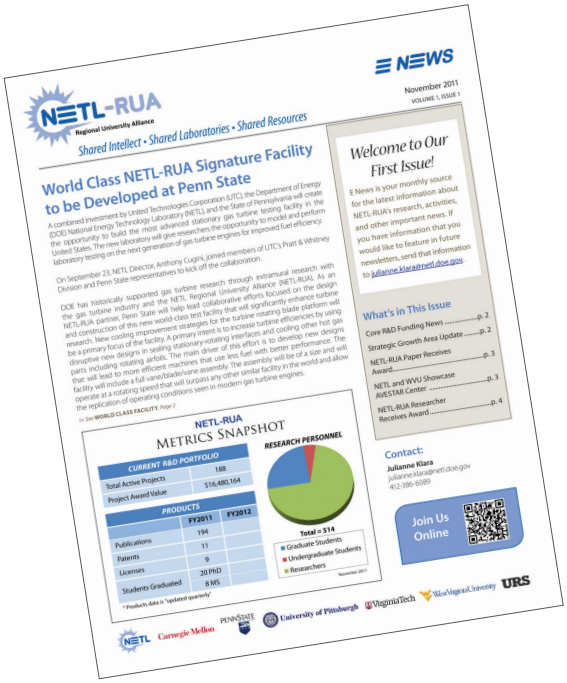
FY2011 Peer Reviewed Publications by NETL-RUA Affiliated Authors

NETL-RUA Member Organization	Number of Publications
CMU	277
NETL	96
PITT	59
PSU	171
URS	9
VT	35
WVU	64
Total	**711**

Citations of FY11 Publications by NETL-RUA Affiliated Authors (as of June 2012)

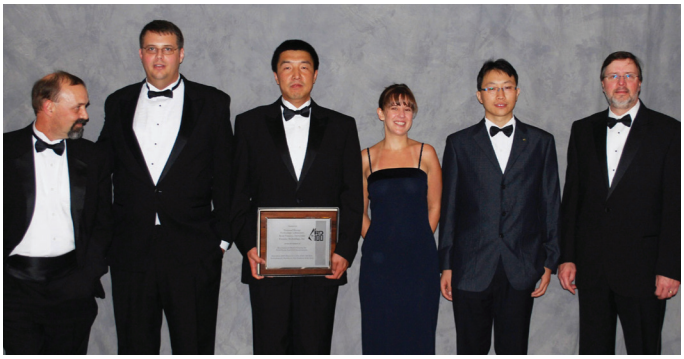
NETL-RUA Member Organization	Papers Cited by Other Peer Reviewed Articles	Additional Cited Reviews, Posters, Presentations, etc.	Total Count
CMU	1591	116	1707
NETL	265	59	324
PITT	252	20	272
PSU	455	43	498
URS	6	2	8
VT	49	9	58
WVU	172	39	211
Total	**2790**	**288**	**3078**

NETL-RUA eNews Newsletter: The first issue was distributed electronically to all NETL-RUA members in November 2011. The monthly newsletter serves as a source of the latest information about NETL-RUA's research activities, as well as other important news.



NETL-RUA eNews Newsletter.

The NETL-RUA Committees: Identified and deployed liaisons to six sister committees in an effort to coordinate and collaborate on committee and organizational efforts. The liaisons provide the operational bridge between activities and projects and act as another conduit for maintaining cohesion in day-to day operations.



Pictured from left to right, Chris Johnson (NETL), Timothy Hall (Faraday), Xingbo Liu (WVU), Heather McCrabb (Faraday), Junwei Wu (Harbin Inst. Tech –China), and Randy Gemmen (NETL) accept the award for their novel SOFC interconnect coating.

Recognition

R&D Magazine R&D 100 Awards

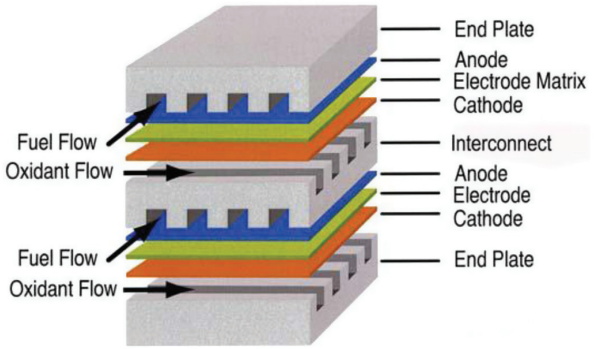
- **Fuel cell interconnect material in fuel cells**: Chris Johnson (NETL), Randy Gemmen (NETL), Xingbo Liu (WVU)

NETL's manganese-cobalt (Mn-Co) coating for SOFC interconnects garnered the laboratory's third 2011 R&D 100 Award. Preventing chromium from evaporating out of the SOFC interconnects increases the stack's lifetime, ultimately making the power generated less expensive for the consumer.

NETL's Chris Johnson and Randy Gemmen, along with WVU researcher Xingbo Liu, decided to pursue $(MnCo)_3O_4$ spinel as the best possible interconnect coating.

The Mn-Co coating offers significant advantages in cost, ease of coating large samples, capability of scaling up for mass production, and environmental friendliness.

This Mn-Co spinel coating was specifically tailored for SOFC interconnects. The coating was designed to prevent the evaporation of chromium from the ferritic stainless-steel-based interconnect while maintaining the electrical conductivity of the interconnect system.



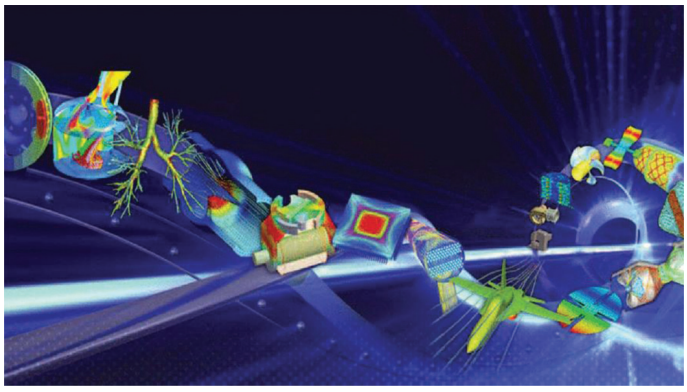
MN - Co Coating for Solid Oxide Fuel Cell Interconnects.

Chromium acts as a poison, increasing the resistance of the interconnect and thus reducing the electrical conductivity and operating lifetime of the fuel cell. Chromium poisoning is one of the major challenges that must be overcome before SOFCs can become commercially viable power sources, and this coating successfully meets this challenge.

The coating was co-developed by NETL and WVU and then transferred to Faraday Technology Inc. for continued development and optimization.

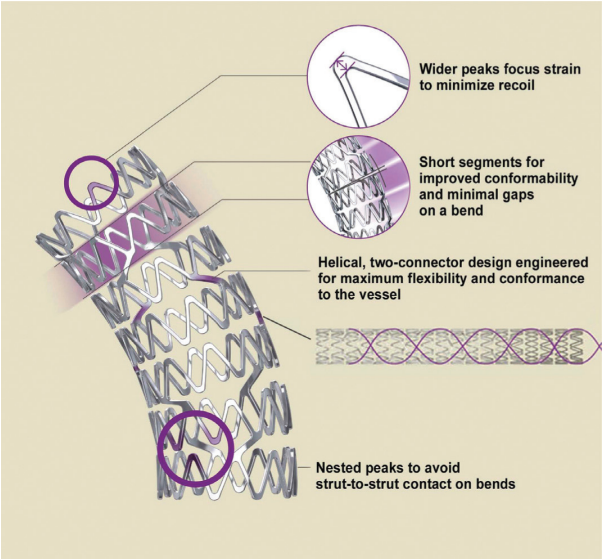
- **Carbon management simulation and visualization**, Stephen Zitney (NETL)

Steve Zitney and his research partners received an award for innovative simulation and visualization technology specific to the evolving needs of carbon management. Companies in the process and energy industries are increasingly relying on sophisticated optimization tools to provide solutions to energy and environmental challenges. NETL's Advanced Process Engineering Co-Simulator (APECS) v2.0 with ANSYS DesignExplorer and ROM Builder tools can aid in the design and optimization of existing and next generation plants for aggressive performance that meets strict economic and environmental objectives. This advanced process simulator reduces the time and cost needed to foster plant innovations by combining process simulation with fast reduced-order models based on high-fidelity equipment-scale.



APECS v2.0 with ANSYS DesignXplorer and ROM Builder.

- **Coronary stent materials**, Paul Jablonski (NETL), Paul Turner (NETL), Ed Argetsinger (NETL); Boston Scientific Corporation.



Coronary stents made from a novel platinum-chromium alloy are more flexible and comfortable than traditional stainless steel stents. The novel alloy was developed by scientists at NETL and BSC. Image courtesy of BSC.

The Novel Platinum/Chromium Alloy for the Manufacture of Improved Coronary Stents is the first austenitic stainless steel formulation with a significant concentration of a highly "radiopaque" element to be produced for the coronary stent industry.

The high radiopacity of the new alloy increases the X-ray visibility of the stent inside a patient. Better visibility results in greater ease and precision of placement of the stent inside the patient's artery and less chance of damage to the artery.

In addition, the greater yield strength of the alloy allowed the stent's designers at Boston Scientific Corporation to make a thinner, more flexible stent that is more easily threaded through the winding path of the artery without causing damage along the way.

The alloy was jointly developed by NETL and Boston Scientific Corporation Inc. After a lengthy series of clinical trials, BSCI succeeded in having the stents approved for sale on November 2, 2009. They were

first marketed in 2010 in Europe and worldwide as the PROMUS® ELEMENT™, selling 206,000 units in Europe, the Middle East, and Africa by December 2010.

On April 25, 2011, the stents, under the TAXUS ION™ label, were approved for sale in the United States.

Since its introduction, sales have exceeded $4 billion and captured a 45 percent share of domestic and about 30% of world coronary stent markets. For more information, visit www.netl.doe.gov/stents.html

2011 Activated Carbon Hall of Fame Award,
Dr. Evan Granite (NETL)

NETL's Evan Granite has been selected by Professional Analytical and Consulting Services, Inc. (PACS) for their Activated Carbon Hall of Fame Award.

The award was presented at the 28th International Activated Carbon Conference in October 2011.

According to PACS, Dr. Granite "has done outstanding work on the subject of mercury recovery from water and air, with special emphasis on the potential one-billion-dollar (USD) market for recovery of mercury from electric power plants burning coal and municipal incinerators practicing waste-to-wealth."

Dr. Evan Granite (NETL), recipient of a 2011 Activated Carbon Hall of Fame Award.

NETL is proud to be a research and technology center where these "energy challenges converge and energy solutions emerge."

2011 Gustav Elrich Award,
Dr. Jinichiro Nakano (URS)

The Gustav Eirich Award was established to recognize outstanding young researchers in the field of refractory materials development. It is intended to promote research excellence among young academics and support innovative ideas in the refractory industry.

Dr. Jinichiro Nakano, a URS scientist at NETL, recipient of a 2011 Gustav Eirich Award.

Awards are given based on the applicant's presentation of environmental aspects, energy, and other resources; the potential for significant impacts to the industry; design and modeling for practical application; and the processing aspects of the development. The goal of the award is to contribute to the long-term success of companies in the refractory production and application industries.

Dr. Nakano was recognized for his NETL research on thermodynamic modeling of coal-petcoke slag compositions and its impact on refractory performance in slagging gasifiers. He received this award at the 54th International Colloquium on Refractories in Aachen, Germany, where he presented his research titled, "A Comprehensive Study of Modern Gasification Slags and Refractories Used in Gasifier to Guide the Development of Novel/Improved Lining Materials."

The research also will be published in an issue of refractories WORLDFORUM—a new technical and scientific journal for the entire refractories sector focusing on production, application, and further development of high-temperature materials. Dr. Nakano is the first U.S.-based researcher to win this award.

SPE International Best Paper Award

to Dr. Dustin McIntyre (DOE), Dr. Jinesh Jain (URS), Shameem Siddiqui (Texas Tech), Krishna Ayyalasomayajula (ORISE), J. P. Singh (Mississippi State), and Fan Yu-Yueh (Mississippi State).

Dual-energy CT-scanning is widely used in the medical industry in DEXA (dual-energy X-ray absorptiometry) systems for measuring bone mineral density after eliminating the effects of X-ray absorption by soft tissues. Dual-energy scanning has also been used quite successfully in fluid flow visualization studies. However, it has not been utilized fully in characterizing reservoir rocks and in particular coal, which, because of its widely variable number of components, provides a challenge for dual-energy CT scanning technology. Development of high purity calibration standards potentially expands use of CT scanning technology on NETL-RUA research projects such as Enhanced Geothermal Systems Research with WVU. This collaboration will help to understand which formations will allow for the identification, through CT identification and quantification, of the most suitable environment for geothermal systems operation and research.

A research paper titled "Analysis of Calibration Materials to Improve Dual-Energy CT Scanning for Petrophysical Applications," co-authored by Dr. Dustin McIntyre of DOE, Dr. Jinesh Jain of URS, and university collaborators [Shameem Siddiqui (Texas Tech); Krishna Ayyalasomayajula (ORISE); JP Singh (Mississippi State); Fang Yu-Yueh (Mississippi State)] describes the steps taken to improve the quality of calibration standards used to perform mineral (and other material) identification applied to the geosciences. CT data are used to measure bulk density and porosity; to quantify heterogeneity; and to make core-to-log comparisons for depth matching and log calibrations. Log calibration is important for correctly identifying mineral contents and generating lithology logs.

Dual-energy CT provides a quick and easy way to calibrate the density and photoelectric logs. The paper has been well received and was awarded the best paper in an annual competition by the Society of Petroleum Engineers (SPE International).

The analysis performed by the NETL-led research team utilizes both inductively coupled plasma optical emission spectroscopy (ICP-OES) and laser induced breakdown spectroscopy (LIBS) to identify and quantify contaminants within the calibration standards.

The identification and quantification of the contaminants allows for the user to adjust the calibration scans to improve the accuracy of the dual energy CT measurements used for material identification in the geosciences.

Dr. Dustin McIntyre (DOE) shown here with the dual-energy CT-scanner.

USGS Director's Award for Exemplary Service

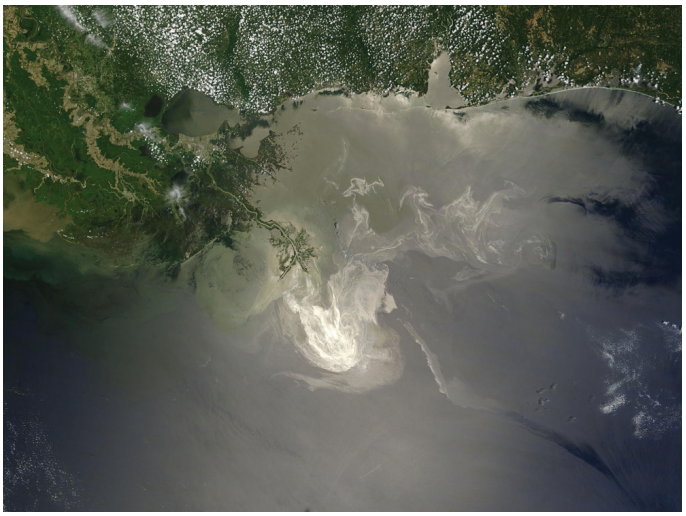
Marcia McNutt, U.S. Geological Survey Director and Chair of the National Incident Command Flow Rate Technical Group (FRTG), recently recognized three NETL employees, Grant Bromhal, George Guthrie, and Frank Shaffer, with the USGS Director's Award for Exemplary Service to the nation in recognition of their contributions during the Deepwater Horizon oil spill response.

Their expertise was called upon to answer important questions, under difficult time constraints and during a period of intense public scrutiny, about the amount of oil leaking from the Macondo Well.

The FRTG's estimate of the oil leak rate was used by the Unified Command to set the level of response in the Gulf of Mexico.

Director McNutt later stated that FRTG's "answers and insights helped guide important decisions and made a very real and positive difference during the response to this unprecedented oil spill event."

She specifically recognized their ability to "work together as true teams, irrespective of organizational affiliations, setting aside personal and professional lives to tackle these challenges."



The Deepwater Horizon oil spill as seen by NASA's Terra satellite on May 24, 2010. The spill was caused by a sea-floor oil gusher that resulted from a drilling rig explosion on April 20, 2010.

Award recipients for Deepwater Horizon oil spill in the Gulf of Mexico efforts.

Secretary of Energy Achievement Awards

On October 27, 2010, Secretary of Energy Stephen Chu honored the NETL and several partner agencies with two Secretary of Energy Achievement Awards, the highest nonmonetary awards an employee or contractor can receive from DOE. One award recognized NETL and its partners for contributions to the Deepwater Horizon oil spill efforts, which aided in understanding the magnitude of the oil leak from the Macondo Well. The second award honored the NETL-RUA's role in DOE's remediation activities at the Hanford nuclear materials production site in Washington State. An NETL-RUA team of computational fluid dynamics scientists evaluated design specifications for a pulse-jet mixing vessel that must safely process 53 million gallons of liquid nuclear waste as it changes into a stable glass form for permanent storage.

The NETL-RUA Hanford Site Team.

Operations

Governance, Operations, Funding, Resources and Plans for 2012

NETL-RUA at a Glance

The Initial Model

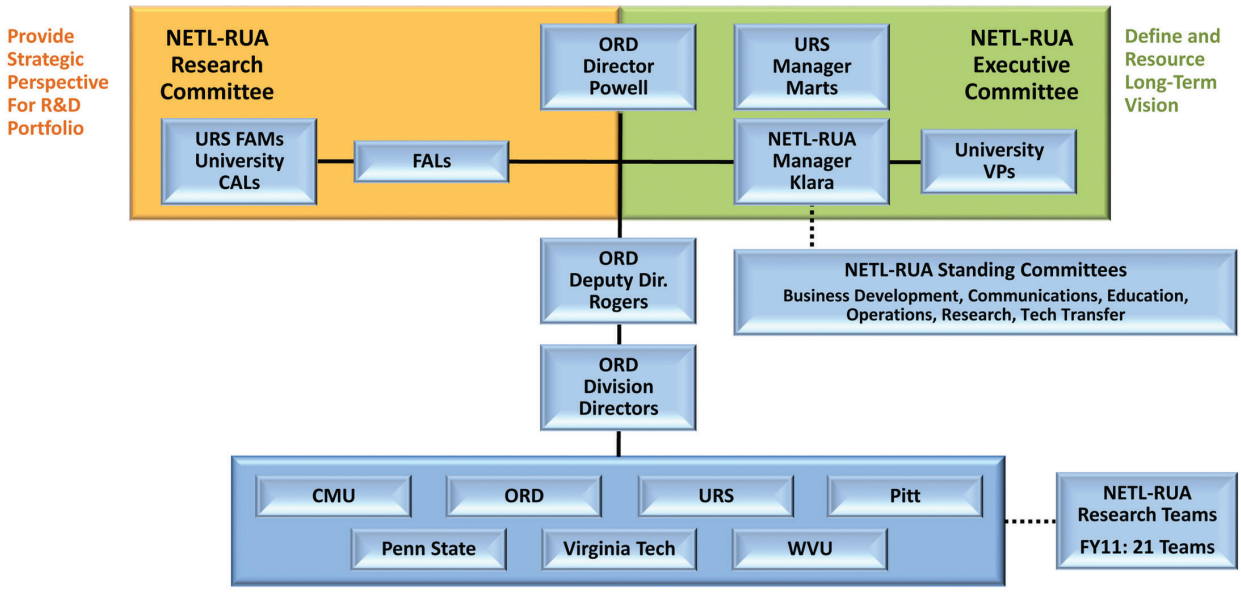
The NETL-RUA continues to grow its structure and operational processes. The member organizations bring considerable and varied experience in administering collections of individual research efforts. But in order to consistently achieve the integrated collaboration of research capabilities among the seven members on a multitude of projects (many linked to research programs), significant operating procedures were needed.

The NETL-RUA research efforts heavily utilize the experience and capabilities of NETL's RES site-support team to implement specific tasks at the universities and within URS. However, to provide guidance to the overall NETL-RUA mission and vision, an initial governance structure was needed. An Executive Committee and functional standing committees, all chaired by ORD staff, were established.

This structure has been advantageous under the initial conditions of the NETL-RUA and, specifically, during its exclusive reliance on DOE/Fossil Energy funding.

However, as strategic requirements lead to a diversification of funding sources, operations are pressed to become more self-starting and more thoroughly Alliance-centric.

In FY2011, the NETL-RUA examined similar government-university-industry research and development collaborations to determine best practices that would be applicable as the NETL-RUA grows. Five areas of best practices were identified and gaps were discovered based on a self-assessment.



NETL-RUA Governance Structure.

Succeeding efforts undertaken in 2011 to develop and implement best practices for the NETL-RUA addressed each of these priority topic areas. These efforts will continue into 2012.

A New Paradigm for Collaboration and Growth

FY2011 marked a significant milestone in the maturation of the NETL-RUA. Out of its strategic push for growth, the NETL-RUA developed a new collaborative research model that will allow it to extend the reach and impact of its R&D portfolio.

Under the direction of its Executive Committee, the NETL-RUA initiated several focused efforts known as "Strategic Growth Areas." The Strategic Growth Areas represent markets in or adjacent to the core fossil energy research portfolio that provide an opportunity to develop the technological platform for this century's energy technology transition. The NETL-RUA Executive committee will jointly fund these initiatives and determine the technical leads .

With the advent of jointly sponsored initiatives and the desire to broaden the scope and effect of the research portfolio, it was necessary to shift from the traditional NETL-RUA research model, which relied solely on NETL sponsorship, to a new model that draws on guidance and funding provided by other NETL-RUA member organizations and clients.

A two-pronged strategy of collaborating for growth is the cornerstone of this model. The first approach is to strengthen NETL-RUA's position as a leader in fossil energy research by placing significant emphasis on accelerating deployment of new energy and environmental technologies to serve as a source of regional economic development and nationwide job creation. NETL-RUA projects are designed to reduce the risk and cost of scale-up by integrating physical and chemical experimental research with computational sciences. The complementary combined capabilities of the NETL-RUA member organizations and those of its partners in industry and sister national laboratories offer a faster pathway for technologies to move from concept to commercialization.

A second strategy is to pursue a broader range of energy and environmental issues and a larger, diversified client base. To accomplish this, the NETL-RUA is leveraging its core competencies toward research needs that represent significant opportunities for growth and provide the potential for making highly significant contributions to new energy strategies and technologies. NETL-RUA teams continue to seek non-traditional funding opportunities such as cooperative programs with industrial partners and large government opportunities such as Innovation Hubs.

NETL-RUA Executive Committee having a strategic planning session.

Resources

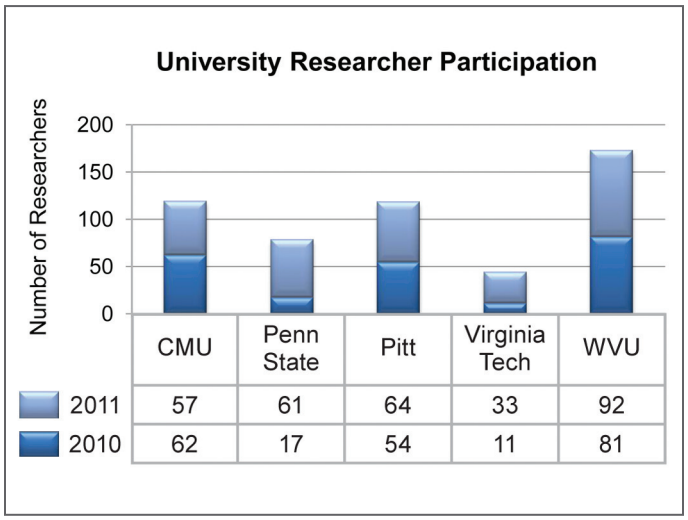
Researchers in the NETL-RUA comprise federal scientists, engineers, and interns from NETL/ORD, faculty and students from the universities, and employees of URS resulting in a collective staff of over 500 researchers.

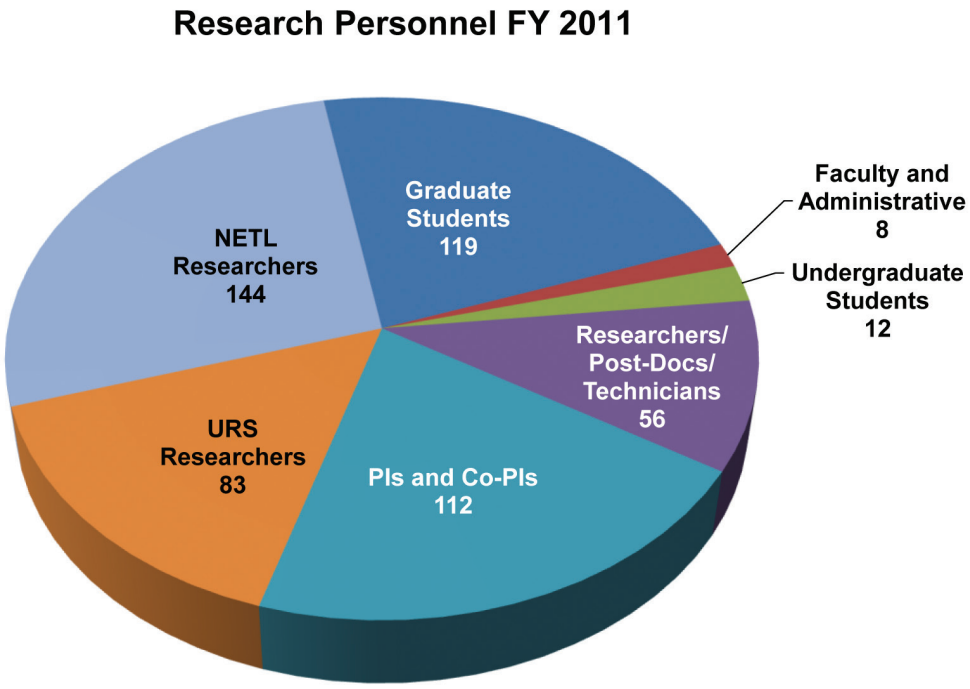
University Researchers	URS Researchers	NETL Researchers	Total RUA Researchers
307	83	144	534

The bar chart represents university researcher particpation within the NETL-RUA for fiscal years 2010 and 2011 and shows the number of researchers has increased during this period.

Three of the universities (Pitt, CMU, and WVU) show a higher number of participants as a result of historical efforts and relationships that have carried over to the NETL-RUA. However, it is evident that the number of researchers from Penn State and Virginia Tech continue to increase as their facilities, capabilities, and faculty expertise are more recognized by NETL-RUA researchers.

The distribution of faculty, post-docs, and students is presented in the pie chart below. There is continued emphasis on involving graduate and undergraduate students in the research to encourage continuing education in science and technology and create the next generation of engineers and scientists that understand the energy challenges facing the nation and the world.





Plans for 2012

FY2012 will see continued emphasis on the growth strategy initiated by the SGAs. This strategy will be accomplished by pursuing funding opportunities and industrial partnerships where NETL-RUA core competencies can offer technological solutions. This will require a more concentrated and coordinated effort among the NETL-RUA members to identify technology that has market application and find target markets that are in need of NETL-RUA's R&D capabilities.

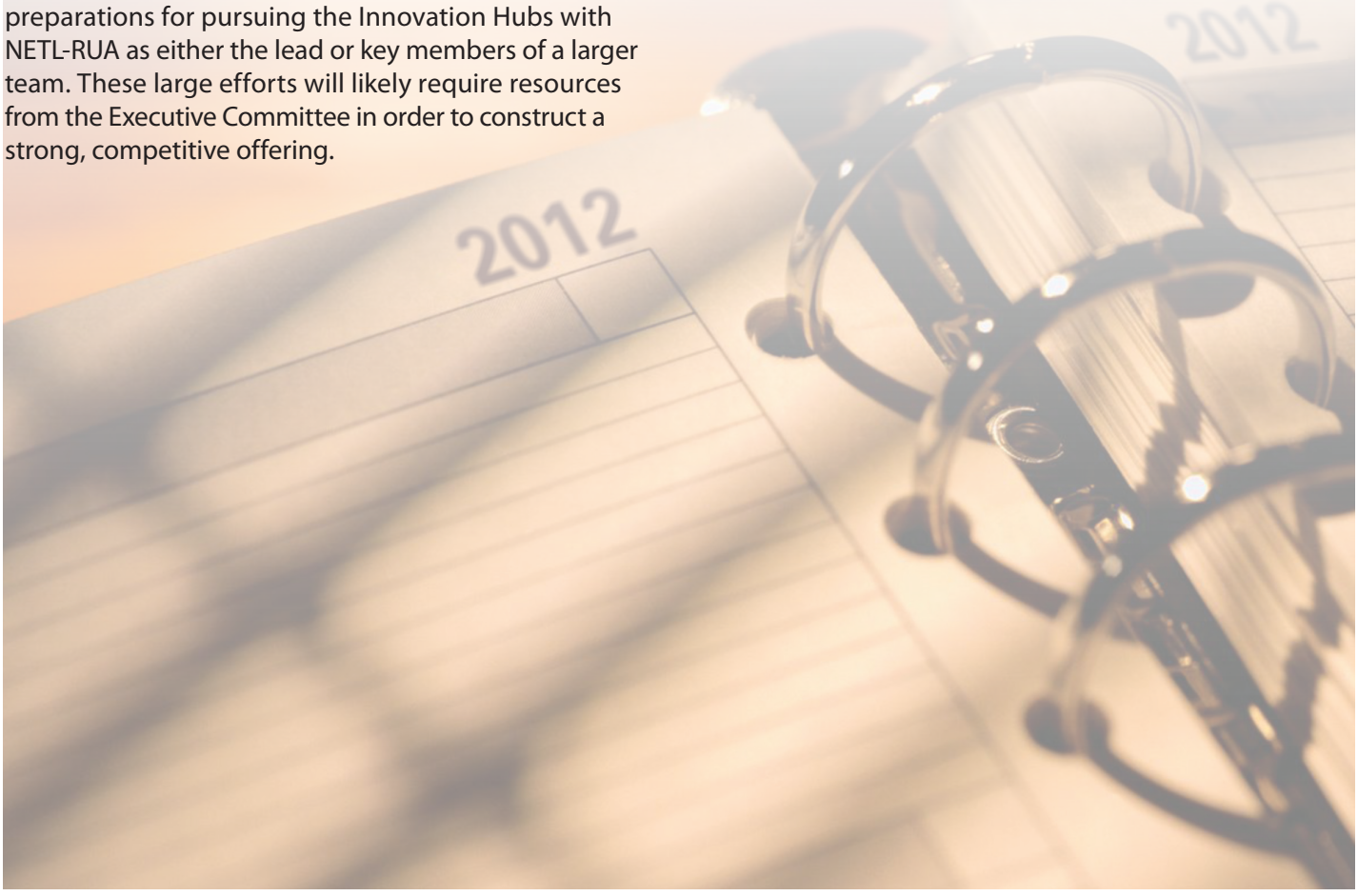
Several important supporting efforts will be needed to ensure that the tools and materials required by NETL-RUA researchers and business development personnel are not only available but designed to successfully pursue and obtain new opportunities.

The federal government has proposed several Innovation Hubs for FY2012. The Grid Technologies, Critical Materials and Rare Earths, and Energy Storage and Batteries SGAs have addressed these opportunities in their workshop white papers. They are making preparations for pursuing the Innovation Hubs with NETL-RUA as either the lead or key members of a larger team. These large efforts will likely require resources from the Executive Committee in order to construct a strong, competitive offering.

Communication among the seven distinct NETL-RUA organizations continues to be a challenge. Though great strides occurred in FY2011 to improve communications, additional efforts to foster collaboration with and improve outreach to NETL-RUA researchers is planned for FY2012 including continued distribution of a monthly electronic newsletter and enhancing the content on the NETL-RUA members-only website. Educational initiatives, beyond the value provided through student research associates, will be investigated in FY2012 including entrepreneurship training and further encouraging undergraduate research.

To enhance visibility of the NETL-RUA and facilitate partnerships with regional industry and manufacturers, the NETL-RUA will hold a technology-focused conference in the fall of 2012 in addition to its 2nd Annual NETL-RUA Spring Meeting.

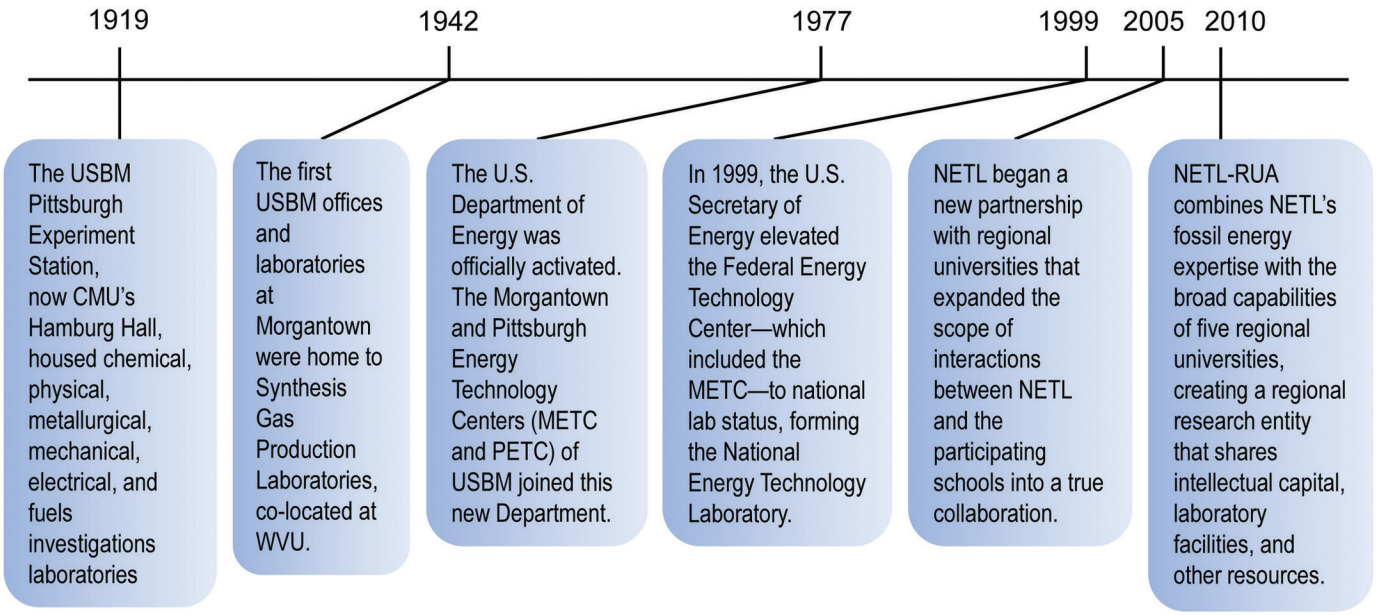
Though much has been accomplished since the NETL-RUA was established, there is still much work to be done. The NETL-RUA will build on this momentum in FY2012 to sustain and accelerate progress.



Appendix A–
NETL-RUA Historical Background

The history of collaborative R&D between NETL-RUA and NETL extends to the initiation of research at the laboratory's R&D campuses. In 1917, the U.S. Bureau of Mines (USBM) opened a facility for coal safety research adjacent to what was then the campus of the Carnegie Institute of Technology (now part of CMU). Energy research at WVU was underway as early as the end of World War II, when experimental facilities for producing synthesis gas from coal were established through a cooperative agreement with USBM. In the ensuing years, CMU, WVU, Pitt, Penn State, and Virginia Tech all performed research funded through NETL's predecessor organizations.

In 2005, NETL began a significant new partnership with regional universities that expanded the scope of interactions between NETL and the participating schools in which university researchers worked side by side with NETL staff and contractors. These collaborative efforts introduced fresh ideas and talent into the research portfolios at each of the institutions. Because it provided a unique opportunity to establish long-term relationships between NETL and university researchers, the collaboration enhanced possibilities for significant breakthroughs in fossil energy grand challenge issues. In its first year, the joint effort conducted less than $3 million in research. However, the collaboration grew significantly, and almost $44 million in research had been performed by the end of 2009.



Appendix B–
NETL-RUA Research Teams and Personnel

Advanced Combustion

NETL Team Lead: Cathy Summers

Name	Affiliation	Title
Beer, Steve	NETL	Physicist
Bullard, Sophie	NETL	Research Chemist
Casleton, Kent	NETL	Physical Scientist
Chorpening, Ben	NETL	Mechanical Engineer
Clark, John	NETL	Material Res. Engineer
Gerdemann, Stephen	NETL	Sr. Chemical Engineer
Hawk, Jeff	NETL	Material Res. Engineer
Holcomb, Gordon	NETL	Material Res. Engineer
Huckaby, David	NETL	Mechanical Engineer
Jablonski, Paul	NETL	Metallurgist
Link, Dirk	NETL	Research Chemist
Matranga, Chris	NETL	Research Chemist
Mei, Joe	NETL	Mechanical Engineer
Ochs, Thomas	NETL	General Engineer
O'Connor, Bill	NETL	Geologist
Oryshchyn, Danylo	NETL	Mechanical Engineer
Shadle, Larry	NETL	Physical Scientist
Straub, Douglas	NETL	Mechanical Engineer
Tylczak, Joe	NETL	Metallurgist
Wen, Youhai	NETL	Material Res. Engineer
Woodside, Charles	NETL	General Engineer
Yip, Joe	NETL	Mechanical Engineer
Ziomek-Moroz, Margaret	NETL	Material Res. Engineer
Carney, Casey	URS	Research Engineer
Carpenter, Stephen	URS	Research Engineer
Gao, Michael	URS	Research Scientist
Hu, Rongxiang (Rachel)	URS	Research Engineer
Jain, Vijay	URS	URS Lead
Lekse, Jonathan	URS	Research Engineer
Montgomery, Christopher	URS	URS Lead
Sears, John	URS	Research Engineer
Tafen, DeNyago	URS	Research Scientist
Williams, Mark	URS	Research Co-Director
Wu, Kaisheng (Kevin)	URS	Research Scientist

Name	Affiliation	Role	University Project Title
Bhavsar, Saurabh K	Pitt	Grad Student	Synthesis and Characterization of Nano-Structured Materials for CO_2 and H_2O Reforming
Meier, Gerald H Yanar, Nazik M Helminiak, Michael A	Pitt	PI Faculty Grad Student	Effects of Deposits Relevant to Oxyfuel Environments on Alloy/Coating Degradation
Haworth, Daniel C Zhao, Xinyu	Penn State	PI Grad Student	PDF-Based Models for Oxy-Coal Combustion
Murayama, Mitsu	Virginia Tech	PI	Multiscale Microstructure Analysis of High-Temperature Structural Materials
Marzouk, Osama A	WVU	PI	CFD support of high-temperature oxy-fuel systems for magneto hydrodynamics (MHD) applications
Marzouk, Osama A	WVU	PI	Oxy-Fuel Pulverized Coal Combustion Simulation and Design

Advanced Gasification

NETL Team Lead: Christopher Guenther

Name	Affiliation	Title
Bennett, James	NETL	General Engineer
Breault, Ron	NETL	General Engineer
Shahnam, Mehrdad	NETL	General Engineer
VanEssendelft, Dirk	NETL	General Engineer
Zitney, Steve	NETL	General Engineer
Jain, Vijay	URS	URS Lead
Mahapatra, Priyadarshi	URS	Research Engineer
Montgomery, Christopher	URS	URS Lead
Means, Nick	URS	Research Engineer
Resnik, Kevin	URS	Research Engineer

Name	Affiliation	Role	University Project Title
Seetharaman, Sridhar Ranjan, Sudhir Kaneko, Tetsuya	CMU	PI Researcher Grad Student	Slag Refractory Interactions During Mixed Carbon Feedstock Gasification in Slagging Gasifiers
Elsworth, Derek Chandra, Divya M	Penn State	PI Grad Student	The Mechanical and Transport Characteristics of Coal-Biomass Mixtures – Application to Dry-Feed Systems for AIGCC
Pisupati, Sarma V Soundarrajan, Tchapda, Aime Hilaire Ngongang	Penn State	PI Grad Student Grad Student	Gasification Coal and Biomass Blends
Battaglia, Francine Deza, Mirka M	Virginia Tech	PI Grad Student	Modeling and predicting biomass fluidization to improve co-gasification
Weiland, Nathan T	WVU	PI	RUA Support for Reducing Syngas Cooler Fouling and Unconverted Carbon Production
Turton, Richard Kasule, Job S	WVU	PI Grad Student	Entrained-Flow Gasification Dynamics
Kang, Bruce S Dodrill, Raphael Zhou, Xin	WVU	PI Grad Student Grad Student	Mechanical Property Evaluation of Torrefied Biomass Materials with Correlation to Grinding Efficiency
Weiland, Nathan T	WVU	PI	RUA Support for Co-gasification Reactions and Kinetics
Turton, Richard Chaudhari, Kiran Pandurang	WVU	PI Grad Student	RUA Support for Development of Coal gasification Kinetics for CFD
Song, Xueyan Palacio, Diego	WVU	PI Researcher	Investigation of microstructure and chemistry origin of corrosion of refractory materials for slagging gasifiers
Seetharaman, Sridhar	CMU	PI	RUA Support for Reducing Syngas Cooler Fouling and Unconverted Carbon Production
Pisupati, Sarma V Krishnamoorthy, Vijyaraghavan	Penn State	PI Grad Student	RUA Support for Reducing Syngas Cooler Fouling and Unconverted Carbon Production
Kuhlman	WVU	PI	RUA Support for Reducing Syngas Cooler Fouling and Unconverted Carbon Production

Advanced Simulation

NETL Team Lead: Christopher Guenther

Name	Affiliation	Title
Miller, David	NETL	Research Engineer
Shadle, Larry	NETL	Physical Scientist
Shaffer, Frank	NETL	General Engineer
Shahnam, Mehrdad	NETL	General Engineer
Zitney, Steve	NETL	General Engineer
Cottrell, Roger	URS	Project Manager
Ma, Jinliang	URS	Research Engineer
Montgomery, Christopher	URS	URS Lead
Nicoletti, Philip	URS	Research Scientist
Robey, Edward	URS	Research Scientist

Name	Affiliation	Role	University Project Title
Rubin, Edward S Zhai, Haibo Borgert, Kyle James Kietzke, Karen Versteeg, Peter L	CMU	PI Post Doc Grad Student Grad Student Grad Student	Integrated Environmental Control Model
Biegler, Lorenz T Dowling, Alex	CMU	PI Graduate Student	Process Synthesis, Analysis and Optimization of Pressure Swing Adsorption (PSA) for CO_2 Capture
Biegler, Lorenz T Lang, Yidong	CMU	PI Faculty	Professional Services for the Carbon Capture Simulation Initiative (CCSI)
Sahinidis, Nick V Chang, Young J	CMU	PI Researcher	Professional Services for the Carbon Capture Simulation Initiative (CCSI)
Nystrom, Nicholas A Urbanek, John Welling, Joel	CMU	Faculty Researcher Researcher	Enabling Multiphase Flow Research
Rubin, Edward S Mantriprada, Hari	CMU	PI Researcher	The Role of Simulation and Modeling in Accelerating CO_2 Capture Technology
Rubin, Edward S	CMU	PI	Carbon Capture Simulation Initiative (CCSI) Project Management
Sahinidis, Nick V Cozad, Alison L	CMU	PI Grad Student	Modular Framework for Analysis and Optimization of Coal-based Fossil Energy Systems with CO_2 Capture
Grossmann, Ignacio E Yang, LinLin	CMU	PI Grad Student	Modular Framework for Design & Optimization of Carbon Capture Systems: Simultaneous Optimization of Flowsheet, Heat Recovery, and Water Network
Tafti, Danesh Gopalakrishnan, Pradeep	Virginia Tech	PI Researcher	Element Method (DEM)
Tafti, Danesh Krishnamurthy, Nagendra Ramesh, Sridharan	Virginia Tech	PI Grad Student Grad Student	Heat and Mass Transfer in Porous CO_2 Sorbent Particles
Bhattacharyya, Debangsu	WVU	PI	Carbon Capture Simulation Initiative (CCSI)
Dietiker, Jean-Francois	WVU	PI	Porting MFIX to GPU Architecture
Dietiker, Jean-Francois	WVU	PI	Improving cut cell technique in MFIX
Bhattacharyya, Debangsu Jones, Dustin D Paul, Prokash	WVU	PI Grad Student Grad Student	IGCC Advanced process control and Sensor placement in an IGCC plant with CO_2 capture

Unconventional Fossil

NETL Team Lead: Jamie Brown

Name	Affiliation	Title
Bromhal, Grant	NETL	General Engineer
Dilmore, Robert	NETL	General Engineer
McIntyre, Dustin	NETL	Mechanical Engineer
McLendon, Bob	NETL	General Engineer
Morreale, Bryan	NETL	General Engineer
Mroz, Tom	NETL	Geologist
Romanov, Slava	NETL	Physical Scientist
Soong, Yee	NETL	Chemical Engineer
Sorescu, Dan	NETL	Research Physicist
Wen, Youhai	NETL	Material Res Engineer
Bruner, Kathy	URS	Research Scientist
Crandall, Dustin	URS	Research Engineer
Lynn, Ron	URS	Specialist
Schuller, Bill	URS	Research Scientist
Siegel, Joel	URS	URS Lead
Tapyrial, Deepak	URS	Research Engineer

Name	Affiliation	Role	University Project Title
Enick, Robert M Baled, Hseen O	Pitt Pitt	PI	EOS and experimental high-temperature, high-pressure ultra-deep reservoir fluid density and viscosity
Enick, Robert M Koronaios, Peter McLendon, William J Pallone, Ashley	Pitt	PI Researcher Grad Student Under Grad	CO_2 soluble surfactants for improved mobility control
Mohaghegh, Shahab D	WVU	PI	Modeling Fluid Flow Behavior in Naturally Fractured Unconventional Reservoirs
Aminian, Kashy Ameri, Samuel	WVU	PI Co-PI	Sample Testing and Analysis using the Precision Petrophysical Analysis Laboratoy (PPAL)
Carr, Timothy R Steptoe, Anne P	WVU	PI Grad Student	Geologic Characterization of the Bakken Shale
Wu, Yue	VCU	Student	EOS and experimental work on high temperature high pressure fluid density and viscosity
McHugh, Mark A	VCU	Co-PI	EOS and experimental high-temperature, high-pressure ultra-deep reservoir fluid density and viscosity
Aminian, Kashy	WVU	PI	Shale Gas Porosity, Permeability, Adsorption, and Effects on net Stress Under Representative Pressures using the WVU Precision Petrophysical Lab

CO_2 Capture

NETL Team Lead: David Berry

Name	Affiliation	Title
Duan, Yuhua	NETL	Physical Scientist
Gray, McMahan	NETL	Physical Scientist
Luebke, David	NETL	General Engineer
Pennline, Hank	NETL	Chemical Engineer
Shadle, Larry	NETL	Physical Scientist
Stekel, Jan	NETL	Physical Scientist
Carpenter, Stephen	URS	Research Engineer
Gao, Michael	URS	Research Scientist
Montgomery, Christopher	URS	URS Lead
Shi, Fan	URS	Research Scientist
Thompson, Robert	URS	Research Scientist
Zandhuis, Paul	URS	Research Scientist

Name	Affiliation	Role	University Project Title
Kitchin, John Alesi, Walter R Demeter, Ethan Landon, James R Lee, Anita	CMU	PI Grad Student Grad Student Grad Student Grad Student	Ion exchange resins as CO_2 sorbents for post-combustion CO_2 capture
Johnson, Karl J Zhang, Bo	Pitt	PI Grad Student	Accurate Control of CO_2 Chemical Reactions with Ionic Liquids Through Cation Composition
Johnson, Karl J Liu, Jinchen	Pitt	PI Researcher	Modeling of Nanoporous Materials for CO_2 Capture
Jordan, Kenneth D Wang, Fanfang Karalti, Ozan Karalti, Sefa Nur	Pitt	PI Post Doc Grad Student Grad Student	Accurate Force Fields for Modeling CO_2 Capture by Ionic Liquids
Enick, Robert M	Pitt	PI	RUA Suppoer for CO_2 philic oligomers and phase change solvents for pre-combustion CO_2 capture
Song, Chunshan Johnson, David Rahman, Atikur	Penn State	PI Researcher Grad Student	A Novel Rapid-Cycle Process for CO_2 Capture from Flue Gas of Coal-fired Power Plants
Song, Chunshan	Penn State	PI	Next Generation Solid Molecular Basket Sorbents with Desired Nano-structure for CO_2 Capture from Flue Gas
Lvov, Serguei Fedkin, Mark V Beck, Justin	Penn State	PI Researcher Grad Student	Electrochemical In-situ Monitoring of Metal Degradation in Carbon Sequestration Processes
Janik, Michael J Gao, Hongwei	Penn State	PI Researcher	High-temperature CO_2 separation from gasifier effluents
Rioux, Robert M	Penn State	PI	Calorimetry/Capacity Analysis of NETL Sorbents
Li, Bingyun Jiang, Bingbing Kish, Vincent Noore, Jabeen	WVU	PI Researcher Tech Tech	Phase Change Amines: Next generation materials for CO_2 capture
Kitchin, John	CMU	PI	ICMI Support for Oxygen Carrier Interaction Studies
Vesper, Dorothy	WVU	PI	ICMI Support for Oxygen Carrier Interaction Studies
Saha, Kringan	WVU	Post Doc	Carbon Capture Simulation Initiative (CSSI) Task Set 2 - Particle and Device Scale Models
Siriwardane, Hema J	WVU	PI	Influence of Geochemical Response during CO_2 Sequestration

CO_2 Storage

NETL Team Lead: Donald Martello

Name	Affiliation	Title
Dilmore, Robert	NETL	General Engineer
Goodman, Angela	NETL	Physical Scientist
Griffith, Craig	NETL	Chemical Engineer
Hedges, Sheila	NETL	Research Chemist
McIntyre, Dustin	NETL	Mechanical Engineer
Romanov, Slava	NETL	Physical Scientist
Smith, Duane	NETL	Physical Science Tech
Soong, Yee	NETL	Chemical Engineer
Crandall, Dustin	URS	Research Engineer
Haljasmaa, Igor	URS	Research Engineer
Ilconich, Jeffrey	URS	URS Lead
Lynn, Ron	URS	Specialist
Sams, Neal	URS	Research Scientist

Name	Affiliation	Role	University Project Title
Small, Mitchell J Popova, Olga H	CMU	PI Grad Student	Refining Small-Scale Estimates of Geological Sequestration Resource Using Site-Specific Estimates of Sequestration Capacity–A Pennsylvania Case Study
Hur, Tae Bong Harbert, William Karimi, Bobak	Pitt	PI Co-PI Grad Student	Investigate basin-specific factors affecting CO_2 storage capacity through U.S. national mapping for un-mineable coal seams identified with storage capacity
Lvov, Serguei Fedkin, Mark V Zhao, Haining	Penn State	PI Researcher Grad Student	Modeling of CO_2 Water Rock Interactions (Experimental Modeling of Phase Equilibria in CO_2-Brine-Rock Systems)
Bodnar, Robert J Rimstidt, J D Capobianco, Ryan Krukowski, Elizabeth Stoakes, Preston	Virginia Tech	PI Co-PI Grad Student Grad Student Grad Student	Volumetric Constraints Associated with Carbon Sequestration in Geological Reservoirs
Carr, Timothy R Donaldson, Kurt Fedorko, Evan Lafone, Frank Sharma, Maneesh Bergerud, Blake Elamin, Abdallah Sesack, Steve	WVU	PI Researcher Researcher Researcher Researcher Grad Student Grad Student Grad Student	NatCarb as a Tool for Resource Assessment
Harbert, William	Pitt	PI	ARRA - Enhanced Geothermal Systems Research

CO_2 Utilization

NETL Team Lead: Charles Taylor

Name	Affiliation	Title
Matranga, Chris	NETL	Research Chemist
Gao, Michael	URS	Research Scientist
Lee, Junseok	URS	Research Scientist
Montgomery, Christopher	URS	URS Lead
Zandhuis, Paul	URS	Research Scientist

Name	Affiliation	Role	University Project Title
Jordan, Kenneth D Al-Saidi, Wissam Abdo Su, Xiaoge	Pitt	PI Faculty Grad Student	Photocatalytic Reduction of CO_2
Scime, Earl E Lindon, Michael Allen	WVU	PI Grad Student	CO_2 to Value Added Chemicals using Low-Temperature Plasma
Ranasingha, Oshadha Underwood, Kylee	WVU	Grad Student Grad Student	Novel Industrial Carbon Management
Natesakhawat, Sittichai	Pitt	PI	Heterogeneous Catalysis of Photoactive Materials
Liang, Shuang	Pitt	Grad Student	Heterogeneous Catalysis of Photoactive Materials

CO_2-Water-Rock Geochemistry

NETL Team Lead: Yee Soong

Name	Affiliation	Title
Baltrus, John	NETL	Research Chemist
Gulliver, Djuna	NETL	General Engineer
Guthrie, George	NETL	Focus Area Manager
Hakala, Ale	NETL	Physical Scientist
Howard, Bret	NETL	Research Chemist
Ilconich, Jeffrey	URS	URS Lead
Lopano, Christina	NETL	Physical Scientist
Romanov, Slava	NETL	Physical Scientist
Carlisle, Kristen	URS	Research Scientist
Myshakin, Eugene	URS	Research Scientist

Name	Affiliation	Role	University Project Title
Karamalidis, Burant, Aniela Parthasarathy, Hariprasad	CMU	PI Grad Student Grad Student	Identify key changes in fluid-based organic composition due to CO_2 and CO_2-water-rock reactions and determine the potential for EPA target contaminant release in major U.S. aquifers potentially affected by carbon sequestration
Lowry, Gregory Gregory, Kelvin B Gulliver, Djuna	CMU	PI Co-PI Grad Student	Identification of Microbial Processes Affecting Storage, Seal Integrity, and Metals Mobility at Carbon Sequestration Sites
Dzombak, David A Hsieh, Ming-Kai	CMU	PI Researcher	Modular Framework for Analysis and Optimization of Existing Plants with Freshwater Minimization
Jordan, Kenneth D Wang, Shuo Zhang, Guozhen	Pitt	PI Post Doc Grad Student	Investigate CO_2 trapping mechanisms in clay minerals using quantum mechanical theory
Bodnar, Robert J Esposito, Rosario	Virginia Tech	PI Grad Student	Volcanic natural analogs for CO_2 sequestration
Yoon, Roe-Hoan Troya, Diego Ma, Juan Niu, Jing	Virginia Tech	PI Faculty Grad Student Grad Student	Mineralization of CO_2 for Sequestration
Burgos, William D Heaney, Peter Liu, Yan Peterson, Kristina Wall, Andrew	Penn State	PI Co-PI Grad Student Grad Student Grad Student	Geochemical transformations caused by CO_2 injection or leakage - Burgos
Rimstidt, J D	Virginia T	PI	Developing Reliable Rate Laws from Mineral-Solution Rate Data: A Database and Data Analysis Strategy
Dzombak, David A Hsieh, Ming-Kai	CMU	PI Researcher	Modular Framework for Analysis and Optimization of Existing Plants with Freshwater Minimization

Energy Storage

NETL Team Lead: David Alman

Name	Affiliation	Title
Manivannan, Ayyakkannu	NETL	General Engineer
Jain, Vijay	URS	URS Lead

Name	Affiliation	Role	University Project Title
Kumta, Prashant Epur, Rigved Kadakia, Karan Beck, Faith R	Pitt	PI Grad Student Grad Student Under Grad	New High Energy Density Magnesium Battery Concepts for Stationary Power Smart Electrical Grids
Kumta, Prashant	Pitt	PI	Energy Storage - EERE Research Support for University of Pittsburgh
Wang, Donghai Chen, Zhongxue Lu, Dongping Song, Zhiping Chen, Shuru Yi, Ran Gordin, Mikhail L	Penn State	PI Researcher Researcher Researcher Grad Student Grad Student Under Grad	New High Energy Density Magnesium Battery Concepts for Stationary Power Smart Electrical Grids

Environmental

NETL Team Lead: Donald Martello

Name	Affiliation	Title
Burse, Debbie	NETL	Engineering Technician
Edenborn, Hank	NETL	Microbiologist
Hammack, Rick	NETL	Physical Scientist
Pekney, Natalie	NETL	General Engineer
Sams, Jim	NETL	Hydrologist
Schroeder, Karl	NETL	Physical Scientist
Veloski, Garret	NETL	Research Chemist
Carlisle, Kristen	URS	Research Scientist
Ference, Bob	URS	Research Scientist
Murin, Timothy	URS	Research Scientist
Siegel, Joel	URS	URS Lead
Tamilia, Joe	URS	Technician

Name	Affiliation	Role	University Project Title
Gregory, Kelvin B Murali Mohan, Arvind	CMU	PI Grad Student	Fate of Naturally Occurring Radioactive Material (NORM) in Flowback and Produced Waters from Natural Gas Development
Donahue, Neil Robinson, Allen Henry, Kaytlin	CMU	PI Co-PI Grad Student	Air-Quality Impacts following Photochemical Oxidation of Emissions from Stationary and Mobile Diesel engines associated with Oil and Natural Gas
Enick, Robert M Kaur, Palwinder	Pitt	PI Researcher	Analysis of Water Samples for Organic Components using LC-Q-TOF Spectroscopy
Stewart, Brian W	Pitt	PI	Management of co-produced waters from the Marcellus Shale: Natural metal isotope tracking of water sources and implications for enhancing efficiency of hydrofrac procedures
Vidic, Radisav D Barbot, Elise Noelle Zhang, Tieyuan	Pitt	PI Researcher Grad Student	Fate of Naturally Occuring Radioactive Material (NORM) in Flowback and Produced Waters from Natural Gas Development
Casson, Leonard W	Pitt	PI	Sabbatical Study and Report, Water Energy Nexus
McCawley, Michael	WVU	PI	Support of Air Sampling for Gas Drilling Operations
Lin, Lian-Shin Park, Ho Il	WVU	PI Researcher	Produced Water Management and Reuse Using Photolysis and Capacitive Deionization
Wood, Petra Becker, Douglas Mizel, Jeremy Sheehan, James	WVU	PI Researcher Grad Student Grad Student	Long-term ecological impacts of O&G activities on avian populations and stream systems in the central Appalachians

Extreme Drilling

NETL Team Lead: Jamie Brown

Name	Affiliation	Title
Edenborn, Hank	NETL	Microbiologist
Gamwo, Isaac	NETL	Chemical Engineer
Hawk, Jeff	NETL	Material Res. Engineer
Thornton, Jimmy	NETL	Division Director ER Division
Tran, Phouc	NETL	Mechanical Engineer
Zhang, Wu	NETL	General Engineer
Ziomek-Moroz, Margaret	NETL	Research Chemist
Cheslock, Jason	URS	Research Engineer
Ilconich, Jeffrey	URS	URS Lead
Lindner, Ernest	URS	Research Engineer
Whipple, Gordon	URS	Research Engineer

Name	Affiliation	Role	University Project Title
Lin, Jeen-Shang Mendoza, Jorge Zhou, Yaneng	Pitt	PI Student Student	Modeling and Verification Discrete and Continuum Analysis of Fragmentation Process of Drilling into HPHT Rocks for Oil Production
Heasley, Keith Mishra, Brijes Zhang, Peng	WVU	PI PI Grad Student	Advanced Rock Mechanics Testing of Rocks Under HTHP

Fuel Cells

NETL Team Lead: Randall Gemmen

Name	Affiliation	Title
Gerdes, Kirk	NETL	General Engineer
Jablonski, Paul	NETL	Metallurgist
Manivannan, Ayyakkannu	NETL	General Engineer
Mantz, Yves	NETL	Physical Scientist
O'Connor, Bill	NETL	Geologist
Ohodnicki, Paul	NETL	General Engineer
Pineault, Richard	NETL	Research Chemist
Surdoval, Wayne	NETL	General Engineer
Tucker, David	NETL	Physical Scientist
Gao, Michael	URS	Research Scientist
Kalapos, Tom	URS	URS Lead
Lapeer, Roger	URS	Engineering Technician
Miller, Nick	URS	Research Engineer
Moore, Kevin	URS	Research Scientist
Nielsen, Benjamin	URS	Research Engineer
Ruehl, Dave	URS	Engineering Technician

Name	Affiliation	Role	University Project Title
Salvador, Paul Chao, Robin	CMU	PI Grad Student	Mesoporous Nanoscale Electrocatalysts SOFC Cathode performance Improvements
Salvador, Paul Picard, Yoosuf	CMU	PI Faculty	Multi Scale Determination of Structural Features in Nano-Composite Electrochemical Materials for Improved SOFCs
Lvov, Serguei Fedkin, Mark V Khurana, Sanchit LaBarbera, Mark	Penn State	PI Researcher Grad Student Grad Student	Electrochemical Evaluation of LMA-SOFC Performance
Messing, Gary L Kupp, Elizabeth R Lee, Haijoon	Penn State	PI Researcher Researcher	Testing and Modeling of the Thermomechanical Behavior and Processing of Infiltrated Cathode Solid Oxide Fuel Cells
Chen, Long-Qing Li, Qun Liang, Linyun	Penn State	PI Researcher Researcher	Phase-field Modeling of Microstructure Evolution and Electrochemical Transport in SOFC Cathodes
Celik, Ismail Pakalapati, S. Raju	WVU	PI Researcher	Integrated Multi-Dimensional, Multi-Scale Cathode Model
Liu, Xingbo Gong, Mingyang Li, Yihong	WVU	PI Researcher Grad Student	Modeling and characterization of fundamental kinetics in SOFC Cathodes
Banta, Larry E Shelton, Michael Buchanan, Matthew Magee, Mark E	WVU	PI Grad Student Under Grad Under Grad	Integrated controls for SOFC/GT Hybrid generation systems
Finklea, Harry O Chen, Yun Chen, Xiaoke	WVU	PI Researcher Grad Student	SOFC electrode structures and reference electrodes.
Sabolsky, Edward M Gandavarapu, Sodith Kumar R	WVU	PI Researcher	Microstructural Engineering of Porous SOFC Cathodes
Song, Xueyan Xiao, Xuezhang	WVU	PI Researcher	TEM Analysis of Materials for Advanced Energy Devices
Wu, Nick Zhi, Mingjia	WVU	PI Researcher	Design and optimization of SOFC cathode architecture

Fuels Conversion

NETL Team Lead: Charles Taylor

Name	Affiliation	Title
Alfonso, Dominic	NETL	Physical Scientist
Baltrus, John	NETL	Research Chemist
Sorescu, Dan	NETL	Research Physicist
Deng, Xingyi	URS	Research Scientist
Gao, Michael	URS	Research Scientist
Shi, Fan	URS	Research Scientist
Zandhuis, Paul	URS	URS Lead

Name	Affiliation	Role	University Project Title
Gellman, Andrew Miller, James B Gumuslu, Gamze Reinicker, Aaron D	CMU	PI Co-PI Grad Student Grad Student	Surface structure sensitivity of FT and RWGS catalysis - High throughput studies
Uffalussy, Karen Jeaneen	Pitt	Researcher	Multifunctional Nanomaterials for Water-Gas-Shift Catalysis in Contaminated Fuel Streams
van Duin, Andrianus C Zou, Chenyu	Penn State	PI Grad Student	Development and application of a ReaxFF reactive force field for Fischer-Tropsch catalysis

Hydrates

NETL Team Lead: Jamie Brown

Name	Affiliation	Title
Rose, Kelly	NETL	Geologist
Rosenbaum, Eilis	NETL	General Engineer
Seol, Yongkoo	NETL	Physical Scientist
Warzinski, Bob	NETL	Research Chemist
Disenhoff, Corrine	URS	Research Scientist
Lui, Yong	URS	Research Engineer
Myshakin, Eugene	URS	Research Scientist

Name	Affiliation	Role	University Project Title
Velaga, Sinatha	WVU	Grad Student	Stability of Gas Hydrates in the Presence of Small Driving Forces
Anderson, Brian Garapati, Nagasree Ryan, Terrence	WVU	PI Grad Student Grad Student	Simulation of the Swapping of CH_4 with CO_2 in Hydrate Systems for Sequestration and Energy
Anderson, Brian Gaddipati, Manohar	WVU	PI Grad Student	Economic Assessment of Hydrate Production
Torres, Marta Hong, Wei Li Kim, Ji Hoon	OSU	PI Grad Student Under Grad	National Gas Hydrates Research Activities
Yoon, Roe-Hoan Cha, Jong-Ho	Virginia Tech	PI Researcher	Evaluation of Hydrate Formation Processes for Treatment of High-Salinity ICS Produced Water

Membranes

NETL Team Lead: David Alman

Name	Affiliation	Title
Dogan, Omer	NETL	Material Res Engineer
Granite, Evan	NETL	Chemical Engineer
Howard, Bret	NETL	Research Chemist
Huckaby, David	NETL	Mechanical Engineer
Luebke, David	NETL	General Engineer
Myers, Christina	NETL	Chemical Engineer
Wen, Youhai	NETL	Material Res Engineer
Albenze, Eric	URS	Research Engineer
Ciocco, Michael	URS	Research Scientist
Culp, Jeffery	URS	Research Scientist
Gao, Michael	URS	Research Scientist
Kalapos, Thomas	URS	URS Lead
Miller, James	URS	Research Engineer
Shi, Wei	URS	Research Scientist
Wickramanayake, Deniye	URS	Research Engineer

Name	Affiliation	Role	University Project Title
Miller, James B Sung, Wilson C	CMU	PI Grad Student	High-Permeance, Poison Tolerant Alloys for Hydrogen Separation Applications
Widom, Michael Huhn, William P	CMU	PI Grad Student	Diffusivity of Hydrogen in Low-Cost Membrane Materials
Nulwala, Hunaid	CMU	PI	New Materials for Energy
Rosi, Nathaniel L Leekyoung, Hwang Li, Tao Sammons, Jessica Annette Song, Chengyi Spore, Alexander B	Pitt	PI Grad Student Grad Student Grad Student Grad Student Grad Student	Optimizing MOFs for Selective CO_2 Capture via Cation Exchange
Achary, Damodaran K	Pitt	PI	NMR spectroscopic studies of Ionic liquids for CO_2 capture and separation
Enick, Robert M	Pitt	PI	CO_2 selective membranes based on CO_2 philic oligomers
Gleeson, Brian M	Pitt	PI	Protective-Scale Evolution and Stability in Complex Environments
Jordan, Kenneth D	Pitt	PI	Computational Support Sorbents and Catalysts of Photoactive Materials
Lewis, James Ranasingha, Oshadha Underwood, Kylee	WVU	PI Grad Student Grad Student	Computational Support Sorbents and Catalysts of Photoactive Materials

Multi-scale, Multi-phase Flow

NETL Team Lead: Yee Soong

Name	Affiliation	Title
McIntyre, Dustin	NETL	Mechanical Engineer
Crandall, Dustin	URS	URS Lead

Name	Affiliation	Role	University Project Title
Li, Li	Penn State	PI	Geochemical transformations caused by CO_2 injection or leakage
Ertekin, Turgay Alexis, Dennis Aslan, Erhan	Penn State	PI Grad Student Grad Student	Advanced Carbon Sequestration Numerical Simulator Designed for Field Applications
Karpyn, Zuleima T Cao, Peilin	Penn State	PI Grad Student	Experimental Investigation of Conditions Affecting Wellbore Integrity due to Chemical Reaction using X-ray microCT imaging
Burbey, Thomas J Zhou, Xue Jun Ward, Jim	Virginia Tech	PI Post Doc Under Grad	Modeling Three-Dimensional Deformation, Flow, Fractures, and Temperature Associated with CO_2 Sequestration
Mohaghegh, Shahab D	WVU	PI	Modeling Fluid Flow Behavior in Naturally Fractured Unconventional Reservoirs
Ertekin, Turgay	Penn State	PI	Numerical Modeling of Carbon Dioxide Injection into Depleted Shale Gas Reservoirs
Li, Li Brunet, Jean-Patrick Leopold Heidari, Peyman	Penn State	PI Researcher Grad Student	Multiphase Reactive Transport Processes Associated with Wellbore Cement Degradation during CO_2 Leakage
Li, Li	Penn State	PI	Development of a Reactive Transport Model for the Evolution of Fracture Properties under Conditions Relevant to CO_2 Sequestration

Quantitative MVA

NETL Team Lead: Donald Martello

Name	Affiliation	Title
Bromhal, Grant	NETL	General Engineer
Brown, Tom	NETL	General Engineer
Burse, Debbie	NETL	Engineering Technician
Cardone, Carol	NETL	Physical Scientist
Dilmore, Robert	NETL	General Engineer
Edenborn, Hank	NETL	Microbiologist
Hakala, Ale	NETL	Physical Scientist
Kutchko, Barbara	NETL	Physical Scientist
Lopano, Christina	NETL	Physical Scientist
Pekney, Natalie	NETL	General Engineer
Rohar, Paul	NETL	Physical Scientist
Schroeder, Karl	NETL	Physical Scientist
Sorescu, Dan	NETL	Research Physicist
Wells, Art	NETL	Research Chemist
Ference, Bob	URS	Research Scientist
Siegel, Joel	URS	URS Lead

Name	Affiliation	Role	University Project Title
Capo, Rosemary C Chapman, Elizabeth C	Pitt	PI Grad Student	Biogeochemical Indicators and processes for development of novel MVA Tools - QMVA
Harbert, William Mur, Alan Delaney, Daniel	Pitt	PI Grad Student Under Grad	3D Reflection Seismic Modeling for Perspective CO_2 Storage Site - NRAP
Stewart, Brian W Achille, Megan Flannery, Kelly M	Pitt	PI Under Grad Under Grad	Development of New Natural Isotope Tracers for Quantative MVA
Wang, Anbo Gong, Jianmin Wang, Yunjing	Virginia Tech	PI Researcher Grad student	Electro-optic CO_2 sensor and wireless network
Gao, Dengliang Weishhans, Andrew	WVU	PI Grad Student	Developing new seismic waveform model regression technologies for improved geologic evaluation for reservoir storage capacity and retention permanence in the subsurface
Sharma, Shikha Sack, Andrea	WVU	PI Grad Student	Tracking CO_2 in complex geochemical and geological settings using stable isotope indicators
Vesper, Dorothy Adams, James P Moore, Johnathan E	WVU	PI Grad Student Grad Student	(Bio)geochemical indicators and processes for development of novel MVA tools: Comparison of CO_2- measurement methods, rare earth element indicators and sensors in complexgeochemical and geological settings
Rauch, Henry W	WVU	PI	Hydrogeologic Monitoring of Aquifiers for NETL Monitoring, Verification and Accounting (MVA) Efforts
Harbert, William	Pitt	PI	Physics Related to MVA

Quantitative Risk Assessment

NETL Team Lead: Angela Goodman

Name	Affiliation	Title
Bromhal, Grant	NETL	General Engineer
Hakala, Ale	NETL	Physical Scientist
Wells, Art	NETL	Research Chemist
Haljasmaa, Igor	URS	Research Engineer
Sams, Neal	URS	Research Scientist
Siegel, Joel	URS	URS Lead

Name	Affiliation	Role	University Project Title
Sahinidis, Nick V Zhang, Yan	CMU	PI Grad Student	Risk Assessment in CO_2 Geologic Sequestration
Small, Mitchell J Nakles, David V	CMU	PI Co-PI	Development of an Integrated Risk Assessment Framework to Support Adaptive Site Management
Capo, Rosemary C Stewart, Brian W Gardiner, James	Pitt	PI Co-PI Grad Student	Natural isotope MVA tools for NRAP strategic monitoring
Blumsack, Seth A Frye, Evan J	Penn State	PI Grad Student	Risk-informed Site Selection for the Long Term Geologic Storage of CO_2
Westman, Erik Sadtler, Daniel A	Virginia Tech	PI Grad Student	Seismic Tomography for Carbon Sequestration Risk Analysis - QMVA
Wilson, Tom H Weber, Matthew	WVU	PI Grad Student	Analysis of Data on Faults and Fractures and Its Application to the Assesment of Potential Migration of Injected CO_2 in the Deep Subsurface, Including Leakage through Primary Seals
Mohaghegh, Shahab D	WVU	PI	Risk Analysis of Carbon Sequestration Projects in the scope of System Analysis
Wilson, Tom H Gao, Dengliang Zhu, Lierong	WVU	PI Faculty Grad Student	Analysis of Data on Faults and Fractures and Its Application to the Assesment of Potential Migration of Injected CO_2 in the Deep Subsurface, Including Leakage through Primary Seals
Gray, Donald D Ogretim, Egemen O	WVU	PI Researcher	Near Surface Modeling of Carbon Dioxide Leakage
Siriwardane, Hema J	WVU	PI	Influence of faults and fractures on reservoir performance, seal integrity, and other subsurface layers
Vesper, Dorothy Moore, Johnathan E	WVU	PI Grad Student	(Bio)geochemical indicators and processes for development of novel MVA tools: Comparison of CO_2-measurement methods, rare earth element indicators and sensors in complex geochemical and geological settings (continuing work)
Small, Mitchell J	CMU	PI	Performance Evaluation and Integration of Multiple Deep Subsurface CO_2 Leak Detection Monitoring Technologies
Brantley, Susan L	Penn State	PI	Developing Reliable Rate Laws from Mineral-Solution Rate Data: A Database and Data Analysis Strategy
Blumsack, Seth A	Penn State	PI	Economic Assessment of CO_2 Storage in Shale
Siriwardane, Hema J	WVU	PI	Numerical and Artificial Intelligence Modeling of Carbon Dioxide Injection into Depleted Shale Gas Reservoirs
Mohaghegh, Shahab D	WVU	PI	Numerical and Artificial Intelligence Modeling of Carbon Dioxide Injection into Depleted Shale Gas Reservoirs

Seal Integrity

NETL Team Lead: Cathy Summers

Name	Affiliation	Title
Huerta, Nic	NETL	Physical Scientist
Kutchko, Barbara	NETL	Physical Scientist
Lopano, Christina	NETL	Physical Scientist
O'Connor, Bill	NETL	Geologist
Strazisar, Brian	NETL	Physical Scientist
Verba, Circe	NETL	Physical Scientist
Crandall, Dustin	URS	Research Engineer
Ilconich, Jeffrey	URS	Research Engineer
Jain, Jinesh	URS	Staff Scientist
Siegel, Joel	URS	URS Lead
Wierzbicki, William	URS	Research Engineer

Name	Affiliation	Role	University Project Title
Dzombak, David A Nakles, David V Zhang, Liwei	CMU	PI Co-PI Grad Student	Acid Gas Interaction with Seal Materials under Geologic Sequestration Conditions
Siriwardane, Hema J Gondle, Rajkumar	WVU	PI Researcher	Use of pressure and displacement signatures to estimate reservoir storage potential and identify possible fault activation in the cap rock during CO_2 injection

Sensors

NETL Team Lead: Randall Gemmen

Name	Affiliation	Title
Woodruff, Steven	NETL	Research Chemist
Buric, Michael	NETL	General Engineer
Chorpening, Ben	NETL	Mechanical Engineer
Ohodnicki, Paul	NETL	General Engineer
Kirby, Travis	URS	Research Engineer

Name	Affiliation	Role	University Project Title
Greve, David W Oppenheim, Irving Chin, Tao-Lun	CMU	PI Co-PI Grad Student	RUA Support for Surface acoustic wave sensor development
Greve, David W	CMU	PI	Support for Solids Flow Measurement Sensor Development at High Temperature for Chemical Looping Combustion
Falk, Joel Biedrzycki, Stephen M	Pitt	PI Grad Student	RUA Support for Raman gas composition monitor
Star, Alex Ding, Mengning	Pitt	PI Grad Student	RUA Support for Synthesis and Characterization of SiC Nanostructures for Sensor Development

Turbines

NETL Team Lead: Randall Gemmen

Name	Affiliation	Title
Alvin, Maryanne	NETL	Division Director
Ferguson, Don	NETL	Mechanical Engineer
Hawk, Jeff	NETL	Material Res Engineer
Holcomb, Gordon	NETL	Material Res Engineer
Jablonski, Paul	NETL	Metallurgist
Strakey, Pete	NETL	Physical Sientist
Straub, Douglas	NETL	Mechanical Engineer
Gao, Michael	URS	Research Scientist
Kalapos, Tom	URS	URS Lead
Robey, Edward	URS	Research Scientist

Name	Affiliation	Role	University Project Title
Seetharaman, Sridhar	CMU	PI	Advanced Characterization of Alloy / Scale Interfaces for Guiding Optimized Surface Stability
Chyu, Minking K Gordon, Ben Siw, Sin Chien	Pitt	PI Grad Student Grad Student	Aerothermal Research for Coal-Gas Based Turbine Systems
Givi, Peyman Pisciuneri, Patrick	Pitt	PI Grad Student	LES-FDF simulations of half-scale Sydney Burner
Gleeson, Brian M	Pitt	PI	Diffusion Barrier Coatings for Achieving Extended Component Service at Ultra-High Temperatures
Meier, Gerald H Lutz, Bradley S	Pitt	PI Grad Student	Strengthening and Oxidation Protection of Nb- and Ta-base Alloys for Ultra-High-Temperature Applications
Santavicca, Dom A Quay, Bryan Kim, Kyutae Samarasinghe, Ramal Mills, Sarah	Penn State	PI Researcher Post Doc Under Grad Tech	Utilization of Exhaust Gas Recirculation for Control of Combustion Instabilities in Gas Turbines
Thole, Karen A Barringer, Michael D	Penn State	PI Researcher	Development of a Rotating Rig to Study Secondary flow Leakages and Aerothermal Cooling
Liu, Zi-Kui Shang, Shun-Li Wang, Jiong	Penn State	PI Researcher Researcher	Computational and Experimental Investigations of Thermodynamic and Physical Properties of Complex Slags in Electro Slag
Vandsburger, Uri Farina, Jordan T Pagliaro, Anthony	Virginia Tech	PI Grad Student Grad Student	Scaling Methods of Combustion Dynamics, Lean Blowout, Flashback and Emissions, for the Design of EGR in Gas Turbines
Ekkad, Srinath Narzary, Diganta Leblanc, Chris	Virginia Tech	PI Researcher Grad Student	Advanced Film Cooling Designs for Reduced Coolant Usage and Improved Overall Cooling Performance for Syngas based Gas Turbines
Celik, Ismail Weiland, Nathan T Posada, Jose Escobar, Sergio	WVU	PI Co-PI Researcher Grad Student	RUA Support for Model Verification and Exhaust Gas Recycle Activity number from CLIN 3 - 3.622.243.001.002
Kang, Bruce S Chou, Chia-Nung Iqbal, Gulfam Otunyo, Dumbi Tannenbaum, Jared	WVU	PI Grad Student Grad Student Grad Student Grad Student	TBC Durability / Damage Assessment of Advanced Turbine Components
Liu, Xingbo	WVU	PI	Corrosion Testing

Appendix C–
FY2011 NETL-RUA Publications

Ai, W.; Kuhlman, J.: *Energy Fuels*, 2011, 25 (2), pp. 708–718 DOI: 10.1021/ef101294f Publication Date (Web): January 20, 2011 2011 American Chemical Society

Alfonso, D.: "Computational Studies of experimentally observed structures of sulfur on metal surfaces," *J. Phys. Chem.* 115, 17077 (2011)

Anderson, B.; Hancock, S.; Wilson, S.; Enger, C.; Collett, T.; Boswell, R.; Hunter, R.: "Formation pressure testing at the Mount Elbert Gas Hydrate Stratigraphic Test Well, Alaska North Slope: Operational summary, history matching, and interpretations," *Marine and Petroleum Geology*, Volume 28, Issue 2, February 2011, Pages 478–492

Anderson, B.; Kurihara, M.; White, M.D.; Moridis, G.J.; Wilson, S.J.; Pooladi-Darvish, M.; Gaddipati, M.; Masuda, Y.; Collett, T.S.; Hunter, R.B.; Haritak, H.; Rose, K.; Boswell, R.: "Regional long-term production modeling from a single well test, Mount Elbert Gas Hydrate Stratigraphic Test Well, Alaska North Slope," *Marine and Petroleum Geology*, Volume 28, Issue 2, February 2011, Pages 493–501, "Thematic Set on Scientific results of the Mount Elbert Gas Hydrate Stratigraphic Test Well," Alaska North Slope

Beck, J.; Lvov, S.; Ziomek-Moroz, M.; Holcomb, G.; Tylczak, J.; Alman, D.: "Electrochemical System to Study Corrosion of Metals in Supercritical CO_2 Fluids," Publisher NACE International Document ID 11380 Content Type Conference Paper CORROSION 2011, March 13–17, 2011, Houston, Texas

Beck, J.; Lvov, S.; Fedkin, M.; Ziomek-Moroz, M.; Holcomb, G.; Tylczak, J.; Alman, D.: "Electrochemical System to Study Corrosion of Metals in Supercritical CO_2 Fluids," CORROSION 2011, March 13–17, 2011, Houston, Texas, 2011. NACE International

Benyahia, S.: "On the Effect of Subgrid Drag Closures," *Industrial & Engineering Chemistry Research*, 49, 11, 5122-5131, June 10, 2011

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Biedrzycki, S.; Buric, M.; Falk, J.; Woodruff, S.: "Optical efficiency in metal-lined capillary waveguide Raman sensors," Proc. SPIE 8028, 80280K (2011); doi:10.1117/12.883074

Buric, M.P.; Chen, K.P.; Falk, J.; Woodruff, S.D.: "Multimode metal-lined capillaries for Raman collection and sensing," *JOSA B*, Vol. 27, Issue 12, pp. 2612–2619 (2010) http://dx.doi.org/10.1364/JOSAB.27.002612

Chen, D.L.; Al-Saidi, W.A.; Johnson, J.K.: "Noble gases on metal surfaces: Insights on adsorption site preference," Phys. Rev. B, 84, 241405(R) (2011)

Cheong, W.Y.; Gellman, A.J.: "Energetics of Chiral Imprinting of Cu(100) by Lysine," *J. Phys. Chem. C*, 2011, 115 (4), pp. 1031–1035

Cozad, A.; Chang, Y.; Sahinidis, N.; Miller, D.C.: Optimization of Carbon Capture Systems Using Surrogate Models of Simulated Processes. Paper 134b presented at 2011 AIChE AnnualMeeting, Minneapolis, MN, October 16–21, 2011

Dillon, S.; Helmick, L.; Miller, H.M.; Johnson, C.; Gemmen, R.; Petrova, R.; Barmak, K.; Gerdes, K.; Rohrer, G.S.; Salvador, P.A.: *Journal of the American Ceramic Society,* Volume 94, Issue 11, pp. 4045–4051, November 2011 DOI: 10.1111/j.1551-2916.2011.04673.x

Ding, M.; Tang, Y.; Gou, P.; Reber, M.J.: "Chemical Sensing with Polyaniline Coated Single-Walled Carbon Nanotubes," *Advanced Materials*, Volume 23, Issue 4, pages 536–540, January 25, 2011

Duan, Y.; Parlinski, K.: "Density functional theory study of the structural, electronic, lattice dynamical, and thermodynamic properties of Li_4SiO_4 and its capability for CO_2 capture," *Phys. Rev. B* 84(2011)104113

Duan, Y.: Sorescu, D.C.; Luebke, D.: "Efficent theoretical screening of good solid sorbents for CO_2 capture applications," Proceedings of 28th International Pittsburgh Coal Conference, Pittsburgh, Sept.12–15, 2011

Fritz, K.; Harris, S.; Edenborn, H.M.; Sams J.: Publication Date 2011 Jan 01, OSTI Identifier OSTI ID: 1011526 Conference: Pennsylvania Academy of Science

Gao, D.: "Latest developments in seismic texture analysis for subsurface structure, facies, and reservoir characterization: A review," *Geophysics*, March–April 2011; v. 76; no. 2; p. W1-W13; DOI: 10.1190/1.3553479

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Harbert, W.; Purcell, C.; Mur, A.: "Seismic reflection data processing of 3-D surveys over an EOR CO_2 injection," Energy Procedia, Volume 4, 2011, pp. 3684–3690, 10th International Conference on Greenhouse Gas Control Technologies, Available online 1 April 2011

Holcomb, G.R.: Fireside Corrosion, 2nd JCOAL/NETL Oxyfuel Workshop, Albany, OR, July 14, 2011.

Holcomb, G.R.; Tylczak, J.: Fireside Corrosion, USC Steering Committee Meeting, Chicago, IL, September 7–8, 2011

Holcomb, G.R.; Tylczak, J.: "Task 2: Materials for Advanced Boiler and Oxy-combustion Systems (NETL-US)," presented at the US-UK Energy RTD Collaboration 2009–2013: Advanced Materials Workshop, Portsmouth, UK, September 8–9, 2011

Holcomb, G.R.; Tylczak, J.: "Task 2: Materials for Advanced Boiler and Oxy-combustion Systems (NETL-US)," presented at the US-UK Energy RTD Collaboration 2009–2013: Advanced Materials Workshop, Portland, OR April 28–29, 2011

Holcomb, G.R.; Tylczak, J.: "Task 1: Steam Oxidation (NETL-US)," presented at the US-UK Energy RTD Collaboration 2009–2013: Advanced Materials Workshop, Portsmouth, UK, September 8–9, 2011

Holcomb, G.R.; Tylczak, J.; Hu, R.: "Materials Performance in USC Steam," Proceedings of the 25th Annual Conference on Fossil Energy Materials, Portland, OR, April 26–28, 2011. http://www.netl.doe.gov/publications/proceedings/11/fem/index.html

Holcomb, G.R.; Tylczak, J.; Hu, R.: "Task 1: Steam Oxidation (NETL-US)," Presented at the US-UK Energy RTD Collaboration 2009–2013: Advanced Materials Workshop, Portland, OR, April 28–29, 2011

Holcomb, G.R.; Tylczak, J.; Meier, G.H.; Yanar, N.M.: Materials Performance in USC Steam, USC Steering Committee Meeting, Chicago, IL, September 7–8, 2011

Holcomb, G.R.; Tylczak, J.; Meier, G.H.; Jung, K.; Mu, N.; Yanar, N. M.; Pettit, F.S.: Fireside Corrosion in Oxy-Fuel Combustion of Coal, presented at the 220th ECS Meeting, High Temperature Corrosion and Materials Chemistry 9: A Symposium in Honor of Professor Robert A. Rapp, Boston, MA, October 9–14, 2011

Hur, T.; Tran, P.; Chyu, M.; Romanov, V.: "Evolution of rheological properties of the nanofluids composed of laponite particles and Mg-Fe layered double hydroxide nanosheets," *Polymer*, Volume 52, Issue 10, 4 May 2011, pp. 2238–2243

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Kauffman, D.; Ohodnicki, P.; Kail, B.; Matranga, C.: "Selective Electrocatalytic Activity of Ligand Stabilized Copper Oxide Nanoparticles," *Journal of Physical Chemistry Letters*, 2011, Vol 2, pgs 2038–2043

Iarikov, D.; Oyama, T.S.: "Supported Room Temperature Ionic Liquid Membranes for CO_2/CH_4 Separation," *Chemical Engineering Journal,* Volume 166, Issue 1, 1 January 2011, pages 401–406

Li, B.; Jiang, B.; Fauth, D.J.; Gray, M.L.; Pennline, H.W.; Richards, G.A.: "Innovative nano-layered solid sorbents for CO_2 capture," *Chem Comm*. 47;1719–21

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Liu, J.; Keskin, S.; Sholl, D.S.; Johnson, J.K.: "Molecular Simulations and Theoretical Predictions for Adsportion and Diffusion of CH_4/H_2 and CO_2/CH_4 Mixtures in ZIFs," *J. Phys. Chem*. C, 2011, 115 (25), pp. 12560–12566, DOI: 10.1021/jp203053h, Publication Date (Web): May 23, 2011, 2011 American Chemical Society

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